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SUPPLEMENTARY MATERIAL FOR MICROFILM EDITION

Table 1. Proton assignment for the cyanide adduct of Ala80cyt *c*. The reported shift values have been measured at 303 K.

residue	HN	α	β	others
Thr–5				
Glu-4				
Phe-3	8.68	4.39	2.64^1, 2.91^2	δ 6.99; ε 7.24; ζ 7.08
Lys–2	6.63	3.84	1.46, 1.58	γ 1.19; δ 1.32; ε 2.89
Ala–1	7.68	3.64	1.27	
Gly1	8.12	3.46^1, 3.65^2		
Ser2	9.44		3.87, 3.65	
Ala3		4.02	1.49	
Lys4	8.26	4.03	1.71, 1.83	ε 3.00
Lys5	7.74	4.12	1.39, 1.75	γ 2.22
Gly6	8.68	3.31^1, 4.03^2		
Ala7	7.94	2.29	1.18	
Thr8	7.18	3.89	4.21	γ 1.24
Leu9	7.93	3.88	1.90, 1.58	δ 0.72, 0.92
Phe10	8.59	3.51	2.59^1, 2.87^2	δ 6.87; ε 7.76, 6.22; ζ 6.40
Lys11	8.15	4.22	1.78, 2.11	ε 3.06
Thr12	7.93	4.32		γ 1.32
Arg13	8.40	4.61	1.66^1,1.43^2	γ 1.77
Cys14	7.59	-0.14	1.88^1	
Leu15	7.70	5.85	1.89^1, 2.30^2	γ 2.24; δ 1.37; 1.96
Gln16	9.50	4.47	2.01, 2.05	γ 2.34, 2.57;ε 6.61^1, 7.21^2
Cys17	9.03	6.09	2.50^2, 4.99^1	
His18	11.05	9.78	7.75^1, 11.94^2	δ1 16.54; δ2 16.1; ε1 -3.4
Thr19	10.52	6.14	5.47	γ 2.28
Val20	9.08	4.83	1.88	γ 0.62, 0.67
Glu21	9.10	4.43	1.98, 2.04	γ 2.19, 2.27
Lys22	8.93	3.48	1.57^2, 1.62^1	γ 0.79^2, 0.94^1; δ 1.16^1; ε 3.00^1
Gly23	9.53	3.85, 4.17		
Gly24	8.38	3.83^2, 4.56^1		
Pro25		3.60	2.43, 2.01	
His26	9.08	5.87	3.65^2, 3.71^1	δ2 7.39; ε1 8.17
Lys27	9.34	5.18	2.80^2, 2.89^1	γ 2.44; δ 2.10^1, 2.53^2; ε 3.62^2, 3.69^1
Val28	7.96	3.61	1.49	γ -0.49^1, 0.86^2
Gly29	9.97	3.88^1, 4.01^2		
Pro30		5.33	1.17, 2.44	γ 1.42, 2.73; δ 3.71
Asn31	12.46	6.39	3.00^2, 3.35^1	δ 8.89^1, 8.01^2
Leu32	9.64	4.54	1.23^2, 1.86^1	γ 4.07; δ -0.87^1, -0.42^2
His33	8.22	4.10	3.27, 3.34	δ2 7.35; ε1 8.22
Gly34	9.09	3.69^1, 3.80^2		

Ile35	6.86	3.39	1.10	γ–CH_3 -0.51; γ -0.10, -0.78; δ -0.28
Phe36	7.57	3.92	2.70, 2.78	δ 6.81; ε 6.17; ζ 6.29
Gly37	8.64	3.71^1, 4.13^2		
Arg38	7.84	4.63	1.98, 1.84	γ 1.71
Gln39	7.75	5.09	1.74, 2.15	
Ser40	8.43	4.42	3.44^2, 4.21^1	
Gly41	7.71			
Gln42	7.85	4.54	1.77, 1.88	γ 2.14, 2.22; ε 6.70^2, 7.34^1
Ala43	8.48	4.51	1.83	
Glu44	8.96	4.30	2.24	γ 2.45, 2.53
Gly45	7.25	3.94, 4.79		
Tyr46	7.17	4.21	1.24^1, 2.29^2	δ 6.69, 6.35; ε 4.85, 5.86; η 9.29
Ser47	6.85	4.33	3.28^2, 3.41^1	
Tyr48	7.89	4.50	2.60, 3.29	δ 7.05, 7.20; ε 6.05, 7.12; η 9.42^a
Thr49	9.28	4.22	4.49	γ 1.32; OH 12.0
Asp50	8.55	4.39	2.54^2, 2.62^1	
Ala51	7.65	4.01	1.44	
Asn52	8.05	4.25	2.62^1, 2.73^2	δ 6.34^2, 7.80^1
Ile53	7.47	3.23	1.78	γ-CH_3 0.87; γ 1.02, 1.68; δ 0.94
Lys54	9.00	3.94	1.85, 1.01	γ 1.58, 1.48
Lys55	7.45	4.00	2.00, 1.96	γ 1.37; δ 2.78
Asn56	7.17	4.28	2.32, 2.97	δ 6.53, 7.43
Val57	7.26	3.76	0.98	γ -0.20^1, 0.41^2
Leu58	8.11	4.13	1.29^1, 1.58^2	γ 0.88; δ 0.67, 0.75
Trp59		4.72	2.04^1, 3.26^2	δ1 6.53; ε3 7.12, ε1 8.19; ζ3 6.58, ζ2 6.73; η2 6.36
Asp60	9.55		2.94, 2.71	
Glu61	9.99	3.34	1.35, 1.35	γ 0.89, 1.14
Asn62	8.13	4.54	2.87^1, 2.92^2	δ 7.11^2, 7.74^1
Asn63	9.43	4.58	2.82, 3.13	δ 6.92, 7.39
Met64	8.71	4.17	1.98^1, 1.53^2	ε -0.41
Ser65	7.53	3.77	3.96, 4.25	
Glu66	7.77	4.15	2.17^1, 2.24^2	γ 2.43^1, 2.63^2
Tyr67	8.76	4.52	3.28^2, 3.52^1	δ 7.25, 7.31; ε 7.77, 7.59; OH 19.3
Leu68	8.83	4.99	1.23^2, 1.73^1	γ 1.35; δ -0.95; -0.54
Thr69	7.97	4.37	4.73	γ 1.52
Asn70	7.68	5.54	3.54, 3.63	
Pro71		6.37	6.10^1, 8.82^2	γ 7.40, 9.47; δ 5.48^2, 5.80^1
Tml72	9.62	5.08	2.15, 2.29	γ 2.56, 2.60; ε 3.73; $(CH_3)_3$ 3.13
Lys73	8.24	4.66	2.26^1, 2.37^2	γ 1.81, 1.86; δ 2.07; ε 3.33
Tyr74	8.45	4.87	4.15^1, 4.37^2	δ 7.87; ε 6.98
Ile75	9.57	4.73	3.15	γ–CH_3 1.02; γ 1.80, 3.04; δ 1.70
Pro76		5.05	2.05, 2.55	γ 2.28; δ 3.80
Gly77	9.11	3.81; 4.41		
Thr78	9.61	4.64	5.08	γ 2.57
Lys79	8.92		2.41^1, 2.48^2	γ -0.22, 0.95; δ 1.34; ε 0.40
Ala80	7.18	-1.52	1.40	
Ala81	5.39	4.05	0.39	

Phe82	6.70		0.36	ζ 6.82; QR 7.60
Gly83	7.54	4.26, 5.22		
Gly84		4.27; 5.11		
Leu85	9.04	4.87	1.62, 1.66	γ 1.51; δ 0.61^1, 0.80^2
Lys86	8.78	4.25	1.98, 2.02	γ 1.67, 1.71; δ 1.88, 1.90; ε 3.22
Lys87	8.93	4.51	1.46, 1.66	ε 3.05
Glu88	9.11			
Lys89	8.74	3.94	1.83, 1.88	γ 1.66, 1.71; δ 1.47, 1.52; ε 2.99
Asp90	6.40	4.20	2.43^1, 2.88^2	
Arg91	7.52	3.53	1.86^1, 2.08^2	γ 1.04; δ 2.37
Asn92	8.59	4.51	2.71	
Asp93	8.52	4.11	2.51^2, 2.58^1	
Leu94	8.31	3.82	1.51, 1.44	γ 1.01; δ 0.17, 0.31
Ile95	8.75	2.92	1.77	γ-CH_3 0.17; γ 0.23; δ 0.60
Thr96	7.90	3.68	4.29	γ 1.14
Tyr97	7.60	4.02	2.83^2, 3.51^1	δ 6.61, 6.44; ε 7.23, 7.00
Leu98	8.93	3.00	0.98, 1.05	γ 1.11; δ -0.63, -0.23
Lys99	8.46	3.26	1.12^2, 1.38^1	γ 0.44^1, 0.70^2; δ 2.44^2, 0.64^1
Lys100	6.46	4.12	1.72, 1.75	γ 1.37; δ 1.60; ε 2.95
Ala101	8.22	3.94	0.53	
Ser102	7.61	4.30	3.28	
Glu103	6.83	4.00	1.94^1, 2.01^2	γ 2.27, 2.32

Heme Assignment[b]

1-CH_3 15.4, 2-Hα 6.3, 2-βCH_3 -0.2, α-meso 4.1, 3-CH_3 11.3, 4-Hα -0.1, 4-CH_3 0.3, β-meso -0.8, 5-CH_3 19.5, 6-Hα 1.8, 6-Hα' 1.6, 6-Hβ 0.2, 7-Hα 6.3, 7-Hα' 1.4, 7-Hβ 0.6, 7-Hβ' 0.8, 8-CH_3 22.5, δ-meso -4.3.

a The resonances were measured at 295 K.
1,2 Refer to stereo-specifically assigned protons.
b. Taken from Bren et al., 1995.

PART I

Experimental NOE intensities used for the structural calculation

Note: an asterisk mark (*) indicates the intensities of the peaks that correspond to two or more protons with degenerate chemical shifts are divided by the number of protons they contain.

-3 PHE				HA	-2	LYS+	HB3	11844.0
HN	-3	PHE	HA	9596.0	HA	-2	LYS+	HG2	19471.2
HN	-3	PHE	HB2	20250.0	HA	-2	LYS+	HD2	14080.0
HN	-3	PHE	HB3	12840.0	HA	-2	LYS+	HE2	2524.0
HN	-3	PHE	CG	1664.5*2	HA	-1	ALA	HN	35930.0
HN	-2	LYS+	HN	670.0	HB2	-2	LYS+	HG2	48970.0
HN	-2	LYS+	HG2	2198.0	HB2	-2	LYS+	HE2	11230.8
HA	-3	PHE	HB2	53701.2	HB2	-1	ALA	HN	19630.0
HA	-3	PHE	HB3	12910.8	HB3	-2	LYS+	HG2	66553.2
HA	-3	PHE	CG	9479.4*2	HB3	-2	LYS+	HE2	11978.4
HA	-2	LYS+	HN	18380.0	HG2	-2	LYS+	HD2	103400.0
HB2	-3	PHE	CG	21425.0*2	HG2	-2	LYS+	HE2	8736.0
HB3	-3	PHE	CG	17180.0*2	HG2	-1	ALA	HN	7336.0
CG	-3	PHE	CZ	26450.0*2*2	HD2	-2	LYS+	HE2	10470.0
CG	-3	PHE	HZ	19560.0*2	-1 ALA				
CG	-2	LYS+	HN	4143.0*2	HN	-1	ALA	HA	13170.0
CG	-2	LYS+	HA	2374.0*2	HN	-1	ALA	QB	32650.0
CG	-1	ALA	HA	193.2*2	HA	-1	ALA	QB	80676.0
CG	61	GLU-	HB2	2371.7*2	HA	1	GLY	HN	18430.0
CG	61	GLU-	HB3	10655.0*2	HA	92	ASN	HB3	5803.6
CG	61	GLU-	HG2	2853.0*2	HA	96	THR	QG2	3847.2
CG	61	GLU-	HG3	1566.0*2	QB	1	GLY	HN	22790.0
CG	92	ASN	HA	4544.4*2	1 GLY				
CG	95	ILE	HB	3572.1*2	HN	1	GLY	HA1	2690.0
CG	95	ILE	QG2	5175.0*2	HN	1	GLY	HA2	23180.0
CG	95	ILE	QD1	3968.2*2	HN	92	ASN	HB3	8949.0
CZ	-3	PHE	HZ	135600.0*2	HN	96	THR	QG2	15240.0
CZ	-1	ALA	HA	5812.8*2	HA1	2	SER	HN	10840.0
CZ	-1	ALA	QB	8195.0*2	HA2	2	SER	HN	9317.0
CZ	61	GLU-	HB2	2863.6*2	HA2	93	ASP-	HA	3911.0
CZ	61	GLU-	HB3	9760.0*2	2 SER				
CZ	61	GLU-	HG2	1009.0*2	HN	2	SER	HB2	3049.0
CZ	61	GLU-	HG3	3126.0*2	HN	2	SER	HB3	5049.0
CZ	92	ASN	HA	10042.2*2	HN	5	LYS+	HB3	1316.0
CZ	92	ASN	HB3	5820.0*2	HN	93	ASP-	HA	6819.0
CZ	95	ILE	HA	1538.5*2	HA	2	SER	HB2	12566.4
CZ	95	ILE	HB	12877.2*2	HA	2	SER	HB3	17110.8
CZ	95	ILE	QG2	11430.0*2	HB3	5	LYS+	HB3	41916.0
CZ	95	ILE	QD1	3310.9*2	HB3	5	LYS+	HG2	7128.2
CZ	96	THR	HN	4533.5*2	3 ALA				
HZ	-1	ALA	HA	20000.4	HA	3	ALA	QB	42280.0
HZ	-1	ALA	QB	15860.0	HA	96	THR	QG2	5939.0
HZ	1	GLY	HN	5235.0	HA	97	TYR	HN	12000.0
HZ	61	GLU-	HG3	7021.0	QB	4	LYS+	HN	11560.0
HZ	92	ASN	HA	7817.0	QB	4	LYS+	HA	7047.0
HZ	95	ILE	HB	5753.2	4 LYS+				
HZ	95	ILE	QG2	10370.0	HN	4	LYS+	HA	13018.0
HZ	96	THR	HN	4265.0	HN	4	LYS+	HB2	11010.0
HZ	96	THR	HA	15649.2	HN	4	LYS+	HB3	4192.0
-2 LYS+					HN	4	LYS+	HE2	770.3
HN	-2	LYS+	HA	10300.0	HN	5	LYS+	HN	951.0
HN	-2	LYS+	HB2	5935.0	HA	4	LYS+	HB2	13860.0
HN	-2	LYS+	HG2	8921.0	HA	4	LYS+	HB3	34130.0
HN	-2	LYS+	HD2	14920.0	HA	5	LYS+	HN	4534.0
HN	-2	LYS+	HE2	2311.0	HA	6	GLY	HN	3254.0
HN	-1	ALA	HN	809.1	HA	7	ALA	HN	4190.0
HA	-2	LYS+	HB2	48207.6	HA	7	ALA	QB	9408.0

HB2	5	LYS+	HN	30630.0
HB3	5	LYS+	HN	4694.0
5 LYS+				
HN	5	LYS+	HA	40950.0
HN	5	LYS+	HB2	6839.0
HN	6	GLY	HN	7902.0
HA	5	LYS+	HB2	10730.0
HA	6	GLY	HN	3277.0
HA	8	THR	HN	2171.0
HB3	5	LYS+	HG2	31382.4
HB3	6	GLY	HN	19250.0
HB3	93	ASP-	HB3	35800.8
HG2	6	GLY	HN	1360.0
HG2	93	ASP-	HB3	32440.8
6 GLY				
HN	6	GLY	HA1	8684.0
HN	6	GLY	HA2	17690.0
HN	7	ALA	HN	13730.0
HN	93	ASP-	HB3	10760.0
HN	97	TYR	HB2	1834.0
HA1	7	ALA	HN	5130.0
HA1	9	LEU	QD2	29761.2
HA1	94	LEU	HA	25586.4
HA2	7	ALA	HN	9481.0
HA2	94	LEU	HA	18463.2
7 ALA				
HN	7	ALA	HA	20280.0
HN	7	ALA	QB	75340.0
HN	8	THR	HN	23970.0
HN	97	TYR	HB2	10794.0
HA	7	ALA	QB	100632.0
HA	10	PHE	HN	4661.0
HA	10	PHE	HB2	7481.9
HA	10	PHE	HB3	29895.6
QB	8	THR	HN	26340.0
8 THR				
HN	8	THR	HA	14010.0
HN	8	THR	HB	52890.0
HN	8	THR	QG2	6984.0
HN	9	LEU	HN	42090.0
HN	11	LYS+	HB2	3350.0
HA	8	THR	HB	12280.8
HA	8	THR	QG2	32790.0
HA	9	LEU	HN	5639.0
HA	11	LYS+	HN	5830.0
HA	11	LYS+	HB2	38547.6
HA	11	LYS+	HB3	7011.0
HB	8	THR	QG2	57766.8
HB	9	LEU	HN	2223.0
HB	12	THR	QG2	4249.0
QG2	9	LEU	HN	6203.0
9 LEU				
HN	9	LEU	HA	19900.0
HN	9	LEU	HB2	11090.0
HN	9	LEU	HB3	19310.0
HN	9	LEU	QD1	11390.0
HN	9	LEU	QD2	7671.0
HN	10	PHE	HN	18760.0
HN	11	LYS+	HN	6684.0
HN	94	LEU	QD1	1440.0
HN	94	LEU	QD2	2442.0
HA	9	LEU	HB2	9559.2
HA	9	LEU	HB3	22990.8
HA	9	LEU	QD1	53496.0
HA	9	LEU	QD2	42048.0
HA	10	PHE	HN	5005.0
HA	13	ARG+	HN	1782.0
HA	13	ARG+	HG2	7644.8
HB2	9	LEU	QD1	18396.0
HB2	9	LEU	QD2	169344.0
HB2	10	PHE	HN	15610.0
HB2	94	LEU	HB3	30470.0
HB2	94	LEU	QD1	7350.0
HB2	94	LEU	QD2	12096.0
HB3	9	LEU	QD1	51460.0
HB3	9	LEU	QD2	18312.0
HB3	10	PHE	HN	1863.0
QD1	10	PHE	HN	555.0
QD1	13	ARG+	HN	1355.0
QD1	13	ARG+	HG2	15450.0
QD1	90	ASP-	HB3	1338.1
QD2	10	PHE	HN	11700.0
QD2	85	LEU	QD1	17942.4
QD2	90	ASP-	HN	750.5
QD2	90	ASP-	HA	57355.2
QD2	90	ASP-	HB3	4515.8
QD2	94	LEU	HN	15250.0
QD2	94	LEU	HB2	46746.0
QD2	94	LEU	HB3	19345.2
QD2	94	LEU	QD1	6456.2
QD2	94	LEU	QD2	7312.2
10 PHE				
HN	10	PHE	HA	20760.0
HN	10	PHE	HB2	40760.0
HN	10	PHE	HB3	25800.0
HN	10	PHE	HD2	1371.0
HN	11	LYS+	HN	18740.0
HN	94	LEU	QD1	8063.0
HN	94	LEU	QD2	11210.0
HA	10	PHE	HB2	26787.6
HA	10	PHE	HB3	16531.2
HA	10	PHE	HD2	20958.0
HA	11	LYS+	HN	4408.0
HA	13	ARG+	HN	2366.0
HA	14	CYSS	HN	7285.0
HA	14	CYSS	HB2	10510.0
HA	94	LEU	QD1	18396.0
HA	94	LEU	QD2	21820.0
HB2	10	PHE	HD2	32986.8
HB2	11	LYS+	HN	3526.0
HB2	94	LEU	QD1	6838.4
HB2	94	LEU	QD2	6569.6
HB3	10	PHE	HD2	21151.2
HB3	11	LYS+	HN	30560.0
HE1	10	PHE	HD2	13498.8
HE1	20	VAL	QG2	4918.0
HE1	98	LEU	QD2	525.8
HZ	10	PHE	HE2	5597.0
HZ	18	HES	HB3	1437.0
HE2	10	PHE	HD2	12800.0
HE2	14	CYSS	HB2	38390.0
HE2	18	HES	QM1	3408.0
HE2	19	THR	HA	4932.0
HE2	20	VAL	QG1	28030.0
HE2	32	LEU	QD1	15350.0
HE2	98	LEU	QD2	2690.0
HD2	14	CYSS	HB2	12950.0
HD2	18	HES	QM1	12060.0
HD2	94	LEU	QD1	12348.0
HD2	94	LEU	QD2	22280.0
HD2	98	LEU	QD1	10780.0
HD2	98	LEU	QD2	9769.2
11 LYS+				
HN	11	LYS+	HA	11360.0
HN	11	LYS+	HB2	52110.0
HN	11	LYS+	HB3	5633.0

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HN	12	THR	HN	18240.0
HA	11	LYS+	HB2	8821.0
HA	11	LYS+	HB3	22117.2
HA	11	LYS+	HE2	15590.4
HA	12	THR	HN	5029.0
HA	15	LEU	HN	11600.0
HA	15	LEU	HA	3075.0
HA	15	LEU	HB2	14305.2
HA	15	LEU	QD2	29164.8
HB2	11	LYS+	HE2	24880.0
HB2	12	THR	HN	15040.0
HB2	12	THR	QG2	14733.6
HB3	11	LYS+	HE2	7070.0
HB3	12	THR	HN	3951.0
HB3	12	THR	QG2	6021.1
12	THR			
HN	12	THR	HA	7126.0
HN	12	THR	QG2	23910.0
HN	13	ARG+	HN	17340.0
HA	12	THR	QG2	39505.2
HA	13	ARG+	HN	2250.0
QG2	13	ARG+	HN	1718.0
13	ARG+			
HN	13	ARG+	HA	5015.1
HN	13	ARG+	HB2	17950.0
HN	13	ARG+	HB3	3620.0
HN	13	ARG+	HG2	14470.0
HN	14	CYSS	HN	65310.0
HN	14	CYSS	HA	798.0
HN	15	LEU	HN	12320.0
HA	13	ARG+	HB2	2025.0
HA	13	ARG+	HB3	27854.4
HB2	14	CYSS	HN	8322.0
HB2	18	HES	HT2A	3098.0
HB2	18	HES	QT2	6202.0
HB3	14	CYSS	HN	4833.0
HB3	18	HES	HT2A	6100.0
HB3	18	HES	QT2	13900.0
HB3	82	PHE	HZ	5411.3
HB3	82	PHE	QR	2289.8*5
14	CYSS			
HN	14	CYSS	HA	10340.0
HN	14	CYSS	HB2	3072.0
HN	15	LEU	HA	593.0
HN	15	LEU	HB2	1268.0
HN	15	LEU	HB3	1432.0
HN	16	GLN	HN	2269.0
HA	14	CYSS	HB2	3370.0
HA	18	HES	HT2A	38080.0
HA	18	HES	HAM	17780.0
HA	18	HES	QM3	16270.0
HB2	18	HES	HB3	1557.0
HB2	18	HES	QM1	2796.0
15	LEU			
HN	15	LEU	HA	20670.0
HN	15	LEU	HB2	32960.0
HN	15	LEU	HB3	37820.0
HN	15	LEU	QD2	12830.0
HN	16	GLN	HN	9088.0
HN	17	CYSS	HN	2433.0
HA	15	LEU	HB2	37833.6
HA	15	LEU	HB3	14523.6
HA	15	LEU	HG	20412.0
HA	15	LEU	QD1	6926.6
HA	15	LEU	QD2	18480.0
HA	16	GLN	HN	2890.0
HA	17	CYSS	HN	2377.0
HA	18	HES	HN	13400.0
HB2	15	LEU	HG	52640.0
HB2	15	LEU	QD1	108780.0
HB2	16	GLN	HN	2260.0
HB3	15	LEU	QD1	25998.0
HB3	15	LEU	QD2	55090.0
HB3	16	GLN	HN	7937.0
HG	15	LEU	QD1	38673.6
HG	15	LEU	QD2	112400.0
HG	16	GLN	HN	13580.0
QD1	16	GLN	HN	2881.0
QD1	19	THR	HA	2499.0
16	GLN			
HN	16	GLN	HA	3245.0
HN	16	GLN	HB2	19500.0
HN	16	GLN	HG2	13250.0
HN	16	GLN	HG3	2760.0
HN	17	CYSS	HN	14110.0
HN	18	HES	HN	3222.0
HN	18	HES	QM3	618.0
HA	16	GLN	HB3	20538.0
HA	16	GLN	HG2	13818.0
HA	16	GLN	HG3	13482.0
HB2	16	GLN	HE21	1806.0
HB2	18	HES	QM3	5136.0
HB3	16	GLN	HG3	110500.0
HG2	16	GLN	HE21	1140.0
HG2	16	GLN	HE22	9081.0
HG2	17	CYSS	HN	6611.0
HG3	16	GLN	HE21	681.0
HG3	18	HES	QT4	9777.0
HE21	18	HES	QT4	890.0
HE22	18	HES	QT4	2762.0
17	CYSS			
HN	17	CYSS	HA	14640.0
HN	18	HES	HN	64970.0
HN	18	HES	QM3	5832.0
HA	17	CYSS	HB2	2559.5
HA	17	CYSS	HB3	15860.0
HA	18	HES	HN	4802.0
HA	27	LYS+	HB2	5189.5
HA	27	LYS+	HB3	5749.0
HA	27	LYS+	HE3	3725.4
HA	28	VAL	HN	7800.0
HA	28	VAL	HB	54690.0
HA	28	VAL	QG1	8451.0
HA	28	VAL	QG2	17190.0
HA	29	GLY	HN	12090.0
HB3	18	HES	HN	5949.0
HB3	18	HES	HT4A	10010.0
HB3	28	VAL	HB	2903.0
HB3	28	VAL	QG1	1885.0
HB3	29	GLY	HN	9958.0
18	HES			
HN	18	HES	HA	14540.0
HN	18	HES	HB2	20000.0
HN	18	HES	HB3	3213.0
HN	19	THR	HN	1064.0
HN	19	THR	QG2	2419.0
HA	18	HES	HB2	12410.0
HA	18	HES	HB3	25110.0
HA	19	THR	HN	60310.0
HA	19	THR	HA	1314.0
HA	27	LYS+	HB2	1169.0
HA	31	ASN	HA	7524.0
HB2	19	THR	HN	8217.0
HB2	32	LEU	QD1	8282.0
HB3	19	THR	HN	16940.0
HB3	19	THR	HA	677.0

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HB3	32	LEU	HN	1357.0
HB3	32	LEU	HG	10777
HB3	32	LEU	QD1	13350.0
HB3	32	LEU	QD2	.0
HD1	32	LEU	HG	7580.
HAP71	18	HES	HAP7	252000.0
HAP71	18	HES	HBP7	18975.0
HAP71	18	HES	HBP7	55000.0
HAP71	18	HES	QM8	10500.0
HAP71	52	ASN	HD21	9766.0
HAP71	59	TRP	HE1	1214.0
HAP71	59	TRP	HZ2	20521.2
HAP72	18	HES	HBP7	63000.0
HAP72	18	HES	HBP7	45360.0
HAP72	18	HES	QM8	11000.0
HAP72	52	ASN	HD21	3031.0
HAP72	59	TRP	HE1	7110.0
HAP72	59	TRP	HZ2	33180.0
HAP72	59	TRP	HH2	11140.0
HAP72	67	TYR	HE1	1837.0
HBP73	18	HES	QM8	6682.0
HBP73	32	LEU	QD2	3083.6
HBP73	35	ILE	QD1	17707.2
HBP73	48	TYR	HH	1896.3
HBP73	52	ASN	HD22	2547.2
HBP73	59	TRP	HE1	744.0
HBP73	59	TRP	HZ2	1326.0
HBP74	30	PRO	HG3	9735.0
HBP74	30	PRO	HD2	6465.0
HBP74	48	TYR	HE1	1850.0
HBP74	48	TYR	HH	3392.5
HBP74	52	ASN	HD22	3882.4
QM8	18	HES	HDM	25180.0
QM8	32	LEU	QD1	3501.0
QM8	32	LEU	QD2	7661.0
QM8	35	ILE	QG2	2879.0
QM8	35	ILE	HG12	10880.0
QM8	35	ILE	HG13	3693.0
QM8	35	ILE	QD1	17870.0
QM8	59	TRP	HE1	1741.0
QM8	59	TRP	HZ2	3195.0
QM8	59	TRP	HH2	2648.0
QM8	64	MET	QE	29830.0
QM8	68	LEU	QD1	1212.0
HDM	18	HES	QM1	35170.0
HDM	32	LEU	QD1	6624.0
HDM	32	LEU	QD2	5667.0
HDM	68	LEU	QD1	7208.0
HDM	68	LEU	QD2	3944.0
HDM	98	LEU	QD1	1603.0
QM1	18	HES	QT2	8280.0
QM1	32	LEU	QD1	22300.0
QM1	32	LEU	QD2	3558.0
QM1	68	LEU	HG	2200.0
QM1	68	LEU	QD1	37360.0
QM1	68	LEU	QD2	48390.0
QM1	94	LEU	QD1	49960.0
QM1	94	LEU	QD2	16120.0
QM1	98	LEU	QD1	38040.0
QM1	98	LEU	QD2	20670.0
HT2A	18	HES	QT2	114000.0
HT2A	18	HES	HAM	24000.0
HT2A	18	HES	QM3	6906.0
QT2	68	LEU	QD1	18110.0
QT2	68	LEU	QD2	32090.0
QT2	82	PHE	HZ	30270.0
QT2	82	PHE	QR	8522.0*5
QT2	85	LEU	QD1	16312.8
QT2	85	LEU	QD2	12658.8
QT2	94	LEU	QD1	8103.5
QT2	94	LEU	QD2	24318.0
HAM	18	HES	QM3	25400.0
HAM	82	PHE	HB2	10280.0
QM3	18	HES	HT4A	7000.0
QM3	18	HES	QT4	21210.0
QM3	82	PHE	HB2	10400.0
QM3	82	PHE	QR	894.8*5
HT4A	18	HES	QT4	68990.0
HT4A	18	HES	QM5	8045.0
HT4A	28	VAL	QG1	75790.0
HT4A	80	ALA	HA	1084.0
HT4A	81	ALA	HN	6014.0
QT4	28	VAL	QG1	12400.0
QT4	81	ALA	HN	9630.0
HBM	18	HES	QM5	39800.0
HBM	80	ALA	HA	6118.0
HBM	81	ALA	HN	3881.0
QM5	18	HES	HAP6	11410.0
QM5	18	HES	HAP6	30530.0
QM5	18	HES	HBP6	20991.6
QM5	28	VAL	HA	1295.3
QM5	28	VAL	QG1	36300.0
QM5	28	VAL	QG2	3803.0
QM5	29	GLY	HN	2963.0
QM5	29	GLY	HA1	13370.0
QM5	46	TYR	HE2	2595.0
QM5	79	LYS+	HN	5268.0
QM5	79	LYS+	HB3	13339.2
QM5	79	LYS+	HG2	6087.0
QM5	79	LYS+	HG3	19540.0
QM5	79	LYS+	HD2	6543.0
QM5	79	LYS+	HE3	16110.0
QM5	80	ALA	HN	4411.0
QM5	80	ALA	HA	21290.0
QM5	81	ALA	HN	4358.0
HAP61	18	HES	HBP6	17440.0
HAP61	46	TYR	HE2	10820.0
HAP62	18	HES	HBP6	59380.0
HAP62	46	TYR	HE2	11670.0
HBP63	79	LYS+	HN	13410.0
HBP63	80	ALA	HN	13540.0
HBP63	80	ALA	HA	1798.0
HBP63	80	ALA	QB	83210.4

19 THR

HN	19	THR	HA	14900.0
HN	19	THR	HB	3956.0
HN	19	THR	QG2	13740.0
HN	20	VAL	HN	672.8
HN	27	LYS+	HG3	1603.0
HN	31	ASN	HA	17440.0
HN	32	LEU	HN	12530.0
HA	19	THR	HB	42142.8
HA	19	THR	QG2	47544.0
HA	20	VAL	HN	51290.0
HA	20	VAL	QG1	7843.1
HA	21	GLU-	HN	4775.0
HB	19	THR	QG2	65721.6
HB	20	VAL	HN	23230.0
HB	20	VAL	HB	1709.4
HB	20	VAL	QG1	858.0
HB	21	GLU-	HN	11800.0
HB	24	GLY	HA2	8351.3
HB	31	ASN	HD21	4753.0
HB	31	ASN	HD22	3076.0
QG2	27	LYS+	HE2	23066.4

20 VAL

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HN	20	VAL	HB	22977.0
HN	20	VAL	QG1	43953.0
HN	20	VAL	QG2	8038.5
HN	21	GLU-	HN	43447.0
HN	21	GLU-	HG2	13271.0
HA	20	VAL	HB	22226.4
HA	20	VAL	QG1	8433.6
HA	20	VAL	QG2	14540.4
HB	20	VAL	QG1	37674.0
HB	20	VAL	QG2	60866.4
HB	98	LEU	QD2	82.9
QG1	21	GLU-	HN	22057.0
QG1	32	LEU	QD1	2859.0
QG1	101	ALA	QB	9089.6
QG2	98	LEU	QD1	2160.5
QG2	98	LEU	QD2	21620.0
QG2	102	SER	HN	3585.0
21	GLU-			
HN	21	GLU-	HG2	29520.0
HN	21	GLU-	HG3	28130.0
HN	24	GLY	HA2	1043.0
HN	31	ASN	HD22	2985.0
HA	21	GLU-	HB2	20874.0
HA	21	GLU-	HB3	14246.4
HA	21	GLU-	HG2	2459.5
HA	21	GLU-	HG3	4717.4
HG3	22	LYS+	HN	6145.0
22	LYS+			
HN	22	LYS+	HA	18740.0
HN	22	LYS+	HB2	15960.0
HN	22	LYS+	HB3	8539.0
HN	22	LYS+	HG2	2630.0
HN	22	LYS+	HG3	10720.0
HA	22	LYS+	HB2	8467.2
HA	22	LYS+	HB3	24561.6
HA	22	LYS+	HG2	46695.6
HA	22	LYS+	HG3	39190.0
HA	22	LYS+	HD2	19219.2
HA	23	GLY	HN	20110.0
HA	24	GLY	HN	1823.0
HA	33	HIS	HD2	4520.9
HB2	22	LYS+	HG2	43671.6
HB2	22	LYS+	HD2	14599.2
HB2	22	LYS+	HE3	29727.6
HB3	22	LYS+	HG3	42714.0
HB3	22	LYS+	HD2	37783.2
HB3	22	LYS+	HE3	32650.8
HB3	23	GLY	HN	3535.0
HB3	33	HIS	HD2	1438.0
HB3	33	HIS	HE1	4701.0
HG2	22	LYS+	HD2	36036.0
HG2	22	LYS+	HE3	6226.1
HG2	23	GLY	HN	5500.0
HG2	33	HIS	HD2	2424.0
HG2	33	HIS	HE1	603.0
HG3	22	LYS+	HD2	23562.0
HG3	23	GLY	HN	2140.0
HG3	33	HIS	HD2	2454.0
HG3	33	HIS	HE1	2823.0
HD2	22	LYS+	HE3	19597.2
HD2	23	GLY	HN	3413.0
HD2	33	HIS	HE1	1575.0
23	GLY			
HN	23	GLY	HA2	346.0
HN	24	GLY	HN	3776.0
HN	24	GLY	HA2	700.0
HA1	24	GLY	HN	5392.4
HA2	24	GLY	HN	10972.1
24	GLY			
HN	24	GLY	HA1	3806.5
HN	24	GLY	HA2	7357.0
HN	31	ASN	HD21	3895.0
HN	31	ASN	HD22	9382.0
25	PRO			
HA	25	PRO	HB3	32365.2
HA	26	HIS	HN	3214.0
HB2	26	HIS	HN	2722.0
HB3	25	PRO	HG2	241416.0
HB3	25	PRO	HG3	21831.6
HB3	26	HIS	HN	4261.0
HG3	25	PRO	HD2	104496.0
26	HIS			
HN	26	HIS	HA	3817.0
HN	26	HIS	HB2	4043.0
HN	26	HIS	HB3	1534.0
HA	26	HIS	HB2	13734.0
HA	26	HIS	HB3	17925.6
HA	26	HIS	HD2	3925.3
HA	27	LYS+	HN	24070.0
HA	27	LYS+	HG3	11121.6
HA	30	PRO	HA	13658.4
HA	31	ASN	HN	11060.0
HA	31	ASN	HB2	6388.2
HA	31	ASN	HB3	4431.8
HB2	26	HIS	HD2	11121.6
HB2	30	PRO	HA	6949.0
HB2	31	ASN	HN	488.0
HB2	46	TYR	HD1	11558.4
HB2	46	TYR	HE1	561.6
HB2	46	TYR	HE2	1712.0
HB3	26	HIS	HD2	16682.4
HB3	30	PRO	HA	11667.6
HB3	46	TYR	HD1	13431.6
HB3	46	TYR	HE2	7374.0
HB3	46	TYR	HD2	4419.2
HD2	30	PRO	HA	854.0
HD2	46	TYR	HA	4207.6
HD2	46	TYR	HB2	3653.2
HE1	30	PRO	HA	3212.2
HE1	30	PRO	HB2	4332.0
HE1	30	PRO	HB3	3581.8
HE1	31	ASN	HN	17100.0
HE1	31	ASN	HB2	9357.6
HE1	31	ASN	HB3	19244.4
HE1	43	ALA	QB	27200.0
HE1	46	TYR	HB2	3780.0
HE1	46	TYR	HB3	6108.0
27	LYS+			
HN	27	LYS+	HA	5593.0
HN	27	LYS+	HB2	9559.0
HN	27	LYS+	HB3	7055.0
HN	27	LYS+	HG3	9619.0
HN	27	LYS+	HD2	1409.0
HN	27	LYS+	HE2	8233.0
HN	27	LYS+	HE3	4177.0
HN	28	VAL	HN	1401.0
HN	29	GLY	HN	5065.0
HN	30	PRO	HA	723.0
HN	31	ASN	HN	993.0
HA	27	LYS+	HB2	13473.6
HA	27	LYS+	HB3	34666.8
HA	27	LYS+	HG3	42268.8
HA	27	LYS+	HD2	12100.0
HA	27	LYS+	HD3	6362.0
HA	27	LYS+	HE2	4860.0
HA	27	LYS+	HE3	5287.0

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HA	28	VAL	HN	1954.0
HA	28	VAL	QG2	3187.8
HB2	27	LYS+	HG3	14288.4
HB2	27	LYS+	HD2	24612.0
HB2	27	LYS+	HE3	23930.0
HB2	28	VAL	HN	22020.0
HB3	27	LYS+	HG3	33507.6
HB3	27	LYS+	HD2	75936.0
HB3	27	LYS+	HE2	4204.2
HB3	27	LYS+	HE3	3667.4
HB3	28	VAL	HN	35900.0
HG3	27	LYS+	HD2	40404.0
HG3	28	VAL	HN	6796.0
HD2	27	LYS+	HE2	6650.3
HD2	27	LYS+	HE3	9075.0
HD3	27	LYS+	HE2	565.0
28 VAL				
HN	28	VAL	HA	15090.0
HN	28	VAL	HB	29190.0
HN	28	VAL	QG1	8189.0
HN	28	VAL	QG2	32870.0
HN	29	GLY	HN	17880.0
HA	28	VAL	HB	11630.0
HA	28	VAL	QG1	47200.0
HA	28	VAL	QG2	52810.8
HA	29	GLY	HN	4583.0
HB	28	VAL	QG1	49490.0
HB	28	VAL	QG2	46905.6
HB	29	GLY	HN	15200.0
HB	29	GLY	HA2	1344.0
QG1	29	GLY	HN	7532.0
29 GLY				
HN	29	GLY	HA1	2281.0
30 PRO				
HA	30	PRO	HB2	52819.2
HA	30	PRO	HB3	37279.2
HA	30	PRO	HG2	3008.0
HA	30	PRO	HG3	3188.0
HA	30	PRO	HD2	1256.0
HA	31	ASN	HN	32680.0
HA	46	TYR	HD1	8887.2
HB2	30	PRO	HG3	3667.0
HB2	31	ASN	HN	5614.0
HB2	43	ALA	QB	17908.8
HB3	30	PRO	HG3	39730.0
HB3	31	ASN	HN	9466.0
HB3	43	ALA	QB	31441.2
HG2	32	LEU	QD2	13920.0
HG2	48	TYR	HH	4083.6
HG3	30	PRO	HD2	9034.0
31 ASN				
HN	31	ASN	HA	12250.0
HN	31	ASN	HB2	18020.0
HN	31	ASN	HB3	23620.0
HN	32	LEU	HN	759.0
HN	43	ALA	QB	3152.0
HA	31	ASN	HB2	36909.6
HA	31	ASN	HB3	12440.0
HA	31	ASN	HD21	9748.0
HA	31	ASN	HD22	5130.0
HA	32	LEU	HN	53660.0
HB2	31	ASN	HD21	14480.0
HB2	31	ASN	HD22	8227.0
HB2	32	LEU	HN	1508.0
HB3	31	ASN	HD21	9635.0
HB3	31	ASN	HD22	2554.0
HD21	32	LEU	HN	8230.0
HD21	33	HIS	HN	291.2
HD22	32	LEU	HN	2790.0
32 LEU				
HN	32	LEU	HA	1862.0
HN	32	LEU	HB2	27550.0
HN	32	LEU	HB3	5234.0
HN	32	LEU	HG	10410.0
HN	32	LEU	QD1	6689.0
HN	32	LEU	QD2	4399.0
HN	33	HIS	HN	14310.0
HA	32	LEU	HB2	10785.6
HA	32	LEU	HB3	28442.4
HA	32	LEU	QD1	5304.6
HA	32	LEU	QD2	41286.0
HA	35	ILE	HB	18320.4
HA	35	ILE	QG2	6985.4
HA	35	ILE	QD1	5684.3
HB2	32	LEU	HG	21117.6
HB2	32	LEU	QD1	20580.0
HB2	32	LEU	QD2	1128.1
HB2	35	ILE	QD1	424.0
HB2	98	LEU	QD2	10040.0
HB3	32	LEU	HG	17800.0
HB3	32	LEU	QD1	52790.0
HB3	32	LEU	QD2	19168.8
HB3	98	LEU	QD1	9724.0
HB3	98	LEU	QD2	17280.0
HG	32	LEU	QD1	21050.0
HG	32	LEU	QD2	20361.6
HG	35	ILE	QG2	3976.6
QD1	98	LEU	QD1	19610.0
QD1	98	LEU	QD2	12500.0
QD2	35	ILE	HB	9413.0
QD2	35	ILE	HG12	49600.0
33 HIS				
HN	33	HIS	HA	11670.0
HN	33	HIS	HB2	13310.0
HN	33	HIS	HB3	10070.0
HA	33	HIS	HB2	10730.0
HA	33	HIS	HB3	19850.0
HA	34	GLY	HN	13080.0
HA	102	SER	HA	28845.6
HB2	33	HIS	HD2	6951.0
HB3	33	HIS	HD2	8601.6
HD2	34	GLY	HA1	502.3
34 GLY				
HN	34	GLY	HA1	25200.0
HN	34	GLY	HA2	313.0
HN	35	ILE	HN	10330.0
HN	103	GLU-	HA	2430.0
HA1	35	ILE	HN	12790.0
35 ILE				
HN	35	ILE	HA	10370.0
HN	35	ILE	HB	47260.0
HN	35	ILE	QG2	33360.0
HN	35	ILE	HG12	5763.0
HN	35	ILE	HG13	7126.0
HN	35	ILE	QD1	7016.0
HA	35	ILE	HB	42820.0
HA	35	ILE	QG2	22110.0
HA	35	ILE	HG12	12583.2
HA	35	ILE	HG13	24750.0
HA	35	ILE	QD1	61420.0
HA	36	PHE	HN	2664.0
HA	38	ARG+	HG2	14666.4
HA	59	TRP	HD1	4175.6
HB	35	ILE	QG2	56926.8
HB	35	ILE	HG12	40610.0
HB	35	ILE	HG13	25640.0

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HB	35	ILE	QD1	49310.0
HB	59	TRP	HD1	555.2
QG2	35	ILE	HG12	10290.0
QG2	35	ILE	HG13	28070.0
QG2	35	ILE	QD1	57370.0
QG2	36	PHE	HN	39860.0
QG2	36	PHE	HA	5658.2
QG2	36	PHE	CG	3769.5*2
QG2	36	PHE	CZ	7265.0*2
QG2	36	PHE	HZ	5072.0
QG2	59	TRP	HD1	759.4
QG2	102	SER	HB2	9886.8
HG12	35	ILE	QD1	42290.0
HG12	59	TRP	HD1	5177.0
HG13	35	ILE	QD1	81120.0
HG13	59	TRP	HD1	11660.0
QD1	59	TRP	HD1	36930.0
QD1	59	TRP	HE1	16190.0
QD1	59	TRP	HZ2	3077.0
QD1	64	MET	QE	13030.0
36 PHE				
HN	36	PHE	HA	11360.0
HN	36	PHE	HB2	29150.0
HN	36	PHE	HB3	4465.0
HN	37	GLY	HN	2199.0
HA	36	PHE	HB2	16090.0
HA	36	PHE	HB3	17967.6
HA	36	PHE	CG	8235.0*2
HA	36	PHE	CZ	1019.0*2
HA	37	GLY	HN	22600.0
HA	38	ARG+	HN	3107.0
HB2	36	PHE	CG	13395.0*2
HB3	36	PHE	CG	12140.0*2
CG	36	PHE	CZ	21504.0*2*2
CG	36	PHE	HZ	29370.0*2
CG	37	GLY	HN	1863.5*2
CG	60	ASP-	HA	9966.6*2
CG	61	GLU-	HN	964.5*2
CG	64	MET	QE	2427.0*2
CG	98	LEU	HB2	2544.8*2
CG	98	LEU	QD1	1308.7*2
CG	99	LYS+	HA	10823.4*2
CG	102	SER	HB2	9105.0*2
CZ	36	PHE	HZ	39719.4*2
CZ	60	ASP-	HA	1270.8*2
CZ	61	GLU-	HN	1638.5*2
CZ	61	GLU-	HA	13830.0*2
CZ	61	GLU-	HB3	4504.0*2
CZ	64	MET	HB2	2303.5*2
CZ	64	MET	HB3	1367.0*2
CZ	64	MET	QE	8980.0*2
CZ	95	ILE	HA	2135.7*2
CZ	95	ILE	QG2	9945.0*2
CZ	98	LEU	HA	1191.1*2
CZ	98	LEU	HB2	20640.0*2
CZ	98	LEU	HB3	12560.0*2
CZ	98	LEU	HG	3690.5*2
CZ	98	LEU	QD1	8590.0*2
CZ	98	LEU	QD2	1674.5*2
CZ	99	LYS+	HN	2887.5*2
CZ	99	LYS+	HA	12028.8*2
HZ	61	GLU-	HA	5367.0
HZ	64	MET	QE	14530.0
HZ	95	ILE	HA	7152.6
HZ	95	ILE	QG2	27680.0
HZ	95	ILE	HG12	5561.0
HZ	98	LEU	HB2	15370.0
HZ	98	LEU	HB3	7898.0
HZ	98	LEU	HG	3110.0
HZ	98	LEU	QD1	16820.0
HZ	98	LEU	QD2	6273.1
HZ	99	LYS+	HN	1277.0
HZ	99	LYS+	HA	2823.2
37 GLY				
HN	37	GLY	HA1	8438.0
HN	37	GLY	HA2	9992.0
HN	38	ARG+	HN	35340.0
HN	58	LEU	QD1	1847.0
HA1	58	LEU	QD1	15657.6
HA2	38	ARG+	HN	1657.0
38 ARG+				
HN	38	ARG+	HB2	5663.0
HN	38	ARG+	HB3	15940.0
HN	38	ARG+	HG2	5879.0
HN	58	LEU	QD1	3618.0
HA	38	ARG+	HB3	4493.2
HA	38	ARG+	HG2	6436.9
HB2	38	ARG+	HG2	152300.0
HG2	59	TRP	HD1	2646.8
39 GLN				
HN	39	GLN	HA	7207.0
HN	39	GLN	HB2	101000.0
HN	39	GLN	HB3	7622.0
HN	42	GLN	HG3	8094.0
HN	59	TRP	HD1	3322.0
HA	39	GLN	HB2	49946.4
HA	39	GLN	HB3	14187.6
HA	40	SER	HN	13190.0
HA	58	LEU	HA	82454.4
HA	58	LEU	HB2	8643.6
HA	58	LEU	HB3	6131.2
HA	58	LEU	QD1	6862.8
HA	59	TRP	HD1	2358.7
HB2	40	SER	HN	27010.0
HB2	56	ASN	HD21	1932.0
HB3	40	SER	HN	4803.0
40 SER				
HN	40	SER	HA	3398.2
HN	40	SER	HB2	5873.0
HN	40	SER	HB3	8424.0
HN	56	ASN	HA	758.0
HN	57	VAL	HN	7510.0
HN	57	VAL	HB	9509.0
HN	57	VAL	QG1	6981.0
HN	57	VAL	QG2	3424.0
HN	58	LEU	HA	2125.0
HN	59	TRP	HD1	653.0
HA	40	SER	HB2	26317.2
HA	40	SER	HB3	51618.0
HA	41	GLY	HN	18630.0
HA	59	TRP	HD1	7181.2
HA	59	TRP	HE1	23759.0
HA	59	TRP	HZ2	1337.0
HB2	41	GLY	HN	3183.0
HB2	57	VAL	QG1	10004.4
HB2	57	VAL	QG2	4399.1
HB2	59	TRP	HZ2	8259.7
HB3	41	GLY	HN	225.0
HB3	57	VAL	HB	17455.2
HB3	57	VAL	QG1	19488.0
HB3	57	VAL	QG2	9130.8
HB3	59	TRP	HE1	2152.0
HB3	59	TRP	HZ2	12020.4
41 GLY				
HN	52	ASN	HD22	2953.0
HN	59	TRP	HE1	12535.0

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42	GLN			
HN	42	GLN	HA	1938.9
HN	42	GLN	HB2	17360.0
HN	42	GLN	HB3	3070.0
HN	42	GLN	HG2	10710.0
HN	42	GLN	HG3	30450.0
HN	43	ALA	HN	17600.0
HN	48	TYR	HE2	8151.0
HA	42	GLN	HB2	34700.4
HA	42	GLN	HB3	7559.0
HA	42	GLN	HG2	14179.2
HA	42	GLN	HG3	31340.4
HA	43	ALA	HN	2630.0
HB2	42	GLN	HG2	42495.6
HB2	42	GLN	HG3	28198.8
HB2	43	ALA	HN	4353.0
HB3	42	GLN	HG2	38472.0
HB3	42	GLN	HG3	18463.2
HG2	42	GLN	HE21	22480.0
HG2	42	GLN	HE22	13700.0
HG3	42	GLN	HE21	7774.0
HG3	42	GLN	HE22	2549.0
43	ALA			
HN	43	ALA	HA	1589.0
HN	43	ALA	QB	35570.0
HN	48	TYR	HD1	2505.0
HN	48	TYR	HE1	1695.0
HN	48	TYR	HE2	3981.0
HN	48	TYR	HH	7468.1
HA	43	ALA	QB	111216.0
HA	44	GLU-	HN	28300.0
QB	44	GLU-	HN	8646.0
QB	48	TYR	HE1	2403.2
QB	48	TYR	HH	7969.5
44	GLU-			
HN	44	GLU-	HA	7128.0
HN	44	GLU-	HB2	67010.0
HN	44	GLU-	HG2	6472.0
HN	44	GLU-	HG3	6989.0
HA	44	GLU-	HB2	64545.6
HA	44	GLU-	HG2	14170.8
HA	44	GLU-	HG3	11533.2
HA	45	GLY	HN	2959.0
HA	46	TYR	HN	2622.0
HB2	45	GLY	HN	5758.0
45	GLY			
HN	45	GLY	HA1	4147.0
HN	45	GLY	HA2	3132.0
HA1	46	TYR	HN	4343.0
HA2	46	TYR	HN	6699.0
46	TYR			
HN	46	TYR	HA	1012.2
HA	46	TYR	HB2	42294.0
HA	46	TYR	HB3	13140.0
HA	46	TYR	HD1	16212.0
HA	47	SER	HN	8387.0
HB2	46	TYR	HD1	13717.2
HB3	46	TYR	HD1	17581.2
HD1	46	TYR	HE1	66603.6
HD1	46	TYR	HE2	25460.4
HE1	46	TYR	HD2	35649.6
HE2	46	TYR	HD2	143724.0
HE2	46	TYR	HH	6149.0
HE2	48	TYR	HA	21184.8
HD2	48	TYR	HA	19891.2
HH	79	LYS+	HE3	1959.0
47	SER			
HN	47	SER	HA	4633.0
HN	47	SER	HB2	5690.0
HN	47	SER	HB3	9881.0
HA	47	SER	HB2	32113.2
HA	47	SER	HB3	76759.2
HA	48	TYR	HN	27590.0
HB2	48	TYR	HN	1604.0
48	TYR			
HN	48	TYR	HA	826.0
HN	48	TYR	HB2	17060.0
HN	48	TYR	HB3	11290.0
HA	48	TYR	HB2	18732.0
HA	48	TYR	HB3	7161.0
HA	49	THR	HN	8034.0
HB2	48	TYR	HD1	12096.0
HB2	48	TYR	HE2	5538.1
HB2	48	TYR	HD2	15338.4
HB2	49	THR	HN	5008.0
HB2	53	ILE	HN	1205.0
HB3	48	TYR	HD1	5437.3
HB3	48	TYR	HE2	7367.6
HB3	48	TYR	HD2	11440.8
HB3	49	THR	HN	7955.0
HD1	48	TYR	HE1	28996.8
HD1	48	TYR	HH	2063.1
HE1	48	TYR	HD2	39345.6
HE1	48	TYR	HH	13225.0
HE2	48	TYR	HH	8450.2
HE2	49	THR	HN	3196.0
49	THR			
HN	49	THR	HA	3172.0
HN	49	THR	HB	3766.0
HN	49	THR	QG2	23310.0
HN	49	THR	HG1	1944.0
HN	52	ASN	HN	2779.0
HN	52	ASN	HB2	6772.0
HN	52	ASN	HB3	6097.0
HA	49	THR	HB	41697.6
HA	49	THR	QG2	83143.2
HA	50	ASP-	HN	47357.0
HB	49	THR	QG2	74944.8
HB	50	ASP-	HN	17859.5
HB	51	ALA	HN	21965.0
HB	51	ALA	QB	4331.9
QG2	50	ASP-	HN	4301.0
QG2	78	THR	HA	19513.2
HG1	52	ASN	HN	14320.0
50	ASP-			
HN	50	ASP-	HA	10562.8
HN	50	ASP-	HB2	23430.0
HN	50	ASP-	HB3	5590.0
HN	51	ALA	HN	11250.0
HA	50	ASP-	HB2	7808.0
HA	50	ASP-	HB3	17136.0
HA	51	ALA	HN	5441.8
HA	53	ILE	HN	2583.0
HA	53	ILE	HB	20034.0
HA	53	ILE	QD1	25410.0
HB2	51	ALA	HN	5905.0
HB3	51	ALA	HN	9990.0
HB3	51	ALA	HA	2043.0
51	ALA			
HN	51	ALA	HA	18160.0
HN	51	ALA	QB	25840.0
HN	52	ASN	HN	12270.0
HA	51	ALA	QB	95960.0
HA	52	ASN	HN	3753.0
HA	54	LYS+	HN	771.1
HA	54	LYS+	HG3	8777.0

HA	75 ILE	QG2	6274.8
QB	52 ASN	HN	22100.0
QB	77 GLY	HA2	21285.6
QB	78 THR	HA	760.4
QB	78 THR	HB	3516.2
52 ASN			
HN	52 ASN	HA	5038.0
HN	52 ASN	HB2	17430.0
HN	52 ASN	HB3	24010.0
HN	53 ILE	HN	12750.0
HN	75 ILE	QG2	2082.0
HA	52 ASN	HB2	38976.0
HA	52 ASN	HB3	10878.0
HA	52 ASN	HD21	4819.0
HA	55 LYS+	HN	8948.0
HA	55 LYS+	HB2	5637.0
HA	55 LYS+	HB3	16090.0
HA	75 ILE	QG2	51156.0
HB2	52 ASN	HD21	16810.0
HB2	52 ASN	HD22	4260.0
HB2	53 ILE	HN	3400.0
HB2	75 ILE	QG2	29601.6
HB3	52 ASN	HD21	9878.0
HB3	52 ASN	HD22	3095.0
HB3	53 ILE	HN	13490.0
HB3	75 ILE	QG2	12087.6
HD21	59 TRP	HZ2	7658.0
HD21	75 ILE	QG2	1957.0
HD22	59 TRP	HE1	1049.0
HD22	59 TRP	HZ2	20450.0
53 ILE			
HN	53 ILE	HA	14220.0
HN	53 ILE	HB	34680.0
HN	53 ILE	QG2	11700.0
HN	53 ILE	HG12	11040.0
HN	53 ILE	HG13	25280.0
HN	53 ILE	QD1	5247.0
HN	54 LYS+	HN	13310.0
HN	54 LYS+	HG2	1775.0
HA	53 ILE	HB	12340.0
HA	53 ILE	QG2	42260.0
HA	53 ILE	HG13	7545.0
HA	53 ILE	QD1	10466.4
HA	54 LYS+	HN	3232.0
HA	55 LYS+	HN	4478.0
HB	53 ILE	QG2	101400.0
HB	53 ILE	HG12	27232.8
HB	53 ILE	QD1	62143.2
HB	54 LYS+	HN	29050.0
HB	54 LYS+	HG2	9304.0
QG2	54 LYS+	HN	13730.0
QG2	54 LYS+	HA	2880.0
QG2	54 LYS+	HG2	30290.0
HG12	53 ILE	QD1	428652.0
HG13	53 ILE	QD1	62974.8
54 LYS+			
HN	54 LYS+	HA	20390.0
HN	54 LYS+	HB2	45560.0
HN	54 LYS+	HB3	3787.0
HN	54 LYS+	HG2	26900.0
HN	54 LYS+	HG3	11280.0
HN	55 LYS+	HN	11370.0
HN	56 ASN	HN	1889.0
HA	54 LYS+	HB2	38910.0
HA	54 LYS+	HG2	21450.0
HA	54 LYS+	HG3	18270.0
HA	55 LYS+	HN	5291.0
HB2	55 LYS+	HN	8222.0
HB3	55 LYS+	HN	1304.0
55 LYS+			
HN	55 LYS+	HA	14990.0
HN	55 LYS+	HB2	14640.0
HN	55 LYS+	HB3	38790.0
HN	55 LYS+	HG2	1313.0
HN	56 ASN	HN	30980.0
HA	55 LYS+	HB2	40470.0
HA	55 LYS+	HB3	12350.0
HA	55 LYS+	HG2	1625.0
HA	56 ASN	HN	4578.0
HB2	55 LYS+	HD2	14054.4
HB2	56 ASN	HN	1286.0
HB2	75 ILE	QG2	31380.0
HB3	56 ASN	HN	2604.0
HB3	57 VAL	HN	3113.0
HB3	57 VAL	QG2	5571.0
HB3	75 ILE	QG2	15440.0
HG2	57 VAL	QG2	31980.0
HG2	75 ILE	QG2	37260.0
HG2	75 ILE	QD1	43580.0
HD2	57 VAL	QG2	8923.0
56 ASN			
HN	56 ASN	HA	34890.0
HN	56 ASN	HB2	18800.0
HN	56 ASN	HB3	4954.0
HA	56 ASN	HB2	25569.6
HA	56 ASN	HB3	11928.0
HA	57 VAL	HN	24390.0
HB2	56 ASN	HD22	94.2
HB3	56 ASN	HD22	2689.0
HN	57 VAL	HA	13540.0
HN	57 VAL	HB	13070.0
HN	57 VAL	QG1	10310.0
HN	57 VAL	QG2	20360.0
HA	57 VAL	HB	10710.0
HA	57 VAL	QG1	16480.8
HA	57 VAL	QG2	20460.0
HA	58 LEU	HN	70430.0
HB	57 VAL	QG1	107000.0
HB	57 VAL	QG2	41610.0
HB	58 LEU	HN	1157.0
HB	59 TRP	HZ2	2442.7
QG1	58 LEU	HN	8919.0
QG1	59 TRP	HA	3522.1
QG1	59 TRP	HE3	8786.0
QG1	59 TRP	HZ3	6828.4
QG1	59 TRP	HZ2	5607.8
QG1	63 ASN	HD21	8463.0
QG1	63 ASN	HD22	3468.0
QG1	74 TYR	CZ	9700.0*2
QG2	58 LEU	HN	12610.0
QG2	59 TRP	HE3	3570.0
QG2	59 TRP	HZ3	3090.0
QG2	59 TRP	HZ2	3103.0
QG2	59 TRP	HH2	2504.0
QG2	63 ASN	HD21	9986.0
QG2	63 ASN	HD22	7602.0
QG2	74 TYR	CG	1763.5*2
QG2	74 TYR	CZ	13350.0*2
QG2	75 ILE	QD1	8180.8
58 LEU			
HN	58 LEU	HA	6048.0
HN	58 LEU	HB2	18590.0
HN	58 LEU	HB3	15950.0
HN	58 LEU	QD1	1025.0
HN	58 LEU	QD2	1754.0

HA	58	LEU	HB2	30580.0
HA	58	LEU	HB3	8916.0
HA	58	LEU	QD1	30256.8
HA	58	LEU	QD2	6851.0
HB2	58	LEU	QD1	26460.0
HB2	58	LEU	QD2	22520.4
HB3	58	LEU	QD1	24850.0
HB3	58	LEU	QD2	58371.6
QD1	60	ASP-	HB3	11530.0
QD2	60	ASP-	HB3	3089.5
59	TRP			
HA	59	TRP	HB2	16153.2
HA	59	TRP	HB3	29509.2
HA	59	TRP	HE3	5671.7
HB2	59	TRP	HD1	9609.6
HB2	59	TRP	HE3	6957.0
HB2	60	ASP-	HN	516.0
HB3	59	TRP	HD1	16245.6
HB3	59	TRP	HE3	23503.2
HB3	60	ASP-	HN	692.0
HD1	59	TRP	HE1	27460.0
HD1	64	MET	QE	1210.0
HE3	59	TRP	HZ3	38690.4
HE3	59	TRP	HH2	9189.6
HE3	60	ASP-	HN	5034.0
HE3	64	MET	HN	9526.0
HE3	64	MET	HA	3359.0
HE3	64	MET	HB2	7027.0
HE3	64	MET	HB3	2955.0
HE3	64	MET	QE	11163.6
HE3	67	TYR	HB2	3040.0
HE1	59	TRP	HZ2	17550.0
HZ3	59	TRP	HZ2	9004.8
HZ3	59	TRP	HH2	63058.8
HZ3	63	ASN	HB3	2023.0
HZ3	64	MET	HN	999.0
HZ3	64	MET	HA	25074.0
HZ3	64	MET	QE	1421.0
HZ3	67	TYR	HN	11220.0
HZ3	67	TYR	HA	4086.6
HZ3	67	TYR	HB2	31332.0
HZ3	67	TYR	HB3	28030.8
HZ3	74	TYR	CG	1228.0*2
HZ2	59	TRP	HH2	59094.0
HZ2	75	ILE	QD1	11088.0
HH2	64	MET	QE	1232.0
HH2	67	TYR	HB2	16330.0
HH2	67	TYR	HB3	14011.2
HH2	74	TYR	CG	13695.0*2
HH2	74	TYR	CZ	838.5*2
HH2	75	ILE	HG12	8986.0
HH2	75	ILE	QD1	23167.2
60	ASP-			
HN	63	ASN	HB3	1043.0
HN	63	ASN	HD21	5165.0
HN	63	ASN	HD22	2933.0
HN	64	MET	HN	722.0
HN	64	MET	HB2	860.0
HA	60	ASP-	HB2	33512.4
HA	60	ASP-	HB3	54036.0
HB2	61	GLU-	HN	18600.0
HB2	62	ASN	HN	6771.0
HB3	61	GLU-	HN	2018.0
61	GLU-			
HN	61	GLU-	HA	13280.0
HN	61	GLU-	HB3	31810.0
HN	61	GLU-	HG2	13280.0
HN	61	GLU-	HG3	11330.0
HN	62	ASN	HN	10860.0
HA	61	GLU-	HB3	30140.0
HA	61	GLU-	HG2	33110.0
HA	61	GLU-	HG3	20420.4
HA	62	ASN	HN	5114.0
HA	64	MET	HN	3707.0
HA	95	ILE	QG2	19714.8
HA	95	ILE	HG12	5845.6
HA	95	ILE	QD1	11860.8
HB2	62	ASN	HN	16260.0
HB2	95	ILE	QG2	9408.0
HB3	61	GLU-	HG2	136700.0
HB3	61	GLU-	HG3	119700.0
HG2	62	ASN	HN	3596.0
HG3	95	ILE	QG2	5733.0
62	ASN			
HN	62	ASN	HB2	20650.0
HN	62	ASN	HB3	11800.0
HN	62	ASN	HD21	4296.0
HN	63	ASN	HN	17300.0
HN	64	MET	HN	2402.0
HA	62	ASN	HB2	6363.8
HA	62	ASN	HB3	17018.4
HB2	62	ASN	HD21	11240.0
HB2	62	ASN	HD22	16110.0
HB3	62	ASN	HD21	8390.0
HB3	62	ASN	HD22	12050.0
HB3	63	ASN	HN	10260.0
63	ASN			
HN	63	ASN	HA	2527.0
HN	63	ASN	HB2	10080.0
HN	63	ASN	HB3	5017.0
HN	64	MET	HN	23330.0
HA	63	ASN	HB2	15355.2
HA	63	ASN	HB3	15372.0
HA	66	GLU-	HB2	8392.4
HA	66	GLU-	HB3	10374.0
HB2	63	ASN	HD21	20920.0
HB2	63	ASN	HD22	26090.0
HB2	64	MET	HN	2826.0
HB3	63	ASN	HD21	6542.0
HB3	63	ASN	HD22	4506.0
HB3	64	MET	HN	2795.0
64	MET			
HN	64	MET	HA	6771.0
HN	64	MET	HB2	45250.0
HN	64	MET	HB3	24490.0
HN	64	MET	QE	5094.0
HN	65	SER	HN	12060.0
HA	67	TYR	HN	5569.0
HA	67	TYR	HB2	11566.8
HB2	64	MET	QE	29360.0
QE	98	LEU	QD1	32516.4
65	SER			
HN	65	SER	HA	7253.0
HN	65	SER	HB2	8959.0
HN	65	SER	HB3	10190.0
HN	66	GLU-	HN	14930.0
HN	67	TYR	HN	832.9
HN	95	ILE	QD1	15770.0
HA	65	SER	HB2	31592.4
HA	65	SER	HB3	7693.6
HA	68	LEU	HN	1185.0
HA	68	LEU	QD2	5024.9
HA	95	ILE	QD1	24788.4
HB2	95	ILE	QD1	37111.2
66	GLU-			
HN	66	GLU-	HA	10110.0

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HN	66	GLU-	HB2	18260.0
HN	66	GLU-	HB3	20330.0
HN	66	GLU-	HG2	2739.0
HN	67	TYR	HN	13940.0
HN	68	LEU	HN	2011.0
HA	66	GLU-	HB2	22772.4
HA	66	GLU-	HB3	14649.6
HA	66	GLU-	HG2	13599.6
HA	66	GLU-	HG3	18992.4
HA	67	TYR	HN	1012.0
HB2	66	GLU-	HG2	35448.0
HB2	67	TYR	HN	5423.0
HB2	74	TYR	CG	2335.0*2
HB2	74	TYR	CZ	3817.0*2
HB3	66	GLU-	HG2	42218.4
HB3	67	TYR	HN	10710.0
HB3	74	TYR	CG	2690.0*2
HB3	74	TYR	CZ	3719.0*2
HG2	74	TYR	CG	7200.0*2
HG2	74	TYR	CZ	4887.0*2
HG3	67	TYR	HN	7516.0
HG3	74	TYR	CG	1609.4*2
67	TYR			
HN	67	TYR	HA	3171.0
HN	67	TYR	HB2	25110.0
HN	67	TYR	HB3	31140.0
HN	74	TYR	CZ	482.6*2
HA	67	TYR	HB2	11062.8
HA	67	TYR	HB3	9693.6
HA	71	PRO	HA	8559.6
HA	74	TYR	CG	5607.0*2
HB2	68	LEU	HN	3528.0
HB2	74	TYR	CG	8260.0*2
HB2	74	TYR	CZ	3063.5*2
HB3	68	LEU	HN	11330.0
HB3	74	TYR	CG	3994.2*2
HD1	67	TYR	HE2	3249.0
HD1	74	TYR	HB3	1153.0
68	LEU			
HN	68	LEU	HA	858.0
HN	68	LEU	HB2	21920.0
HN	68	LEU	HB3	4944.0
HN	68	LEU	HG	9485.0
HN	68	LEU	QD1	2893.0
HN	68	LEU	QD2	15540.0
HN	69	THR	HN	9319.0
HA	68	LEU	HB2	22537.2
HA	68	LEU	HB3	15792.0
HA	68	LEU	HG	13683.6
HA	68	LEU	QD1	44058.0
HA	68	LEU	QD2	7337.4
HA	71	PRO	HG2	298.1
HA	71	PRO	HG3	8526.0
HA	71	PRO	HD3	14473.2
HA	82	PHE	QR	1504.6*5
HB2	68	LEU	QD1	8066.0
HB2	68	LEU	QD2	19970.0
HB2	69	THR	HN	917.0
HB3	68	LEU	QD1	16700.0
HB3	68	LEU	QD2	38665.2
HB3	69	THR	HN	8351.0
HB3	82	PHE	QR	295.4*5
HB3	85	LEU	HN	3482.0
HB3	85	LEU	QD1	2059.7
HG	68	LEU	QD1	27340.0
HG	68	LEU	QD2	45950.0
QD1	71	PRO	HG2	3002.2
QD1	71	PRO	HG3	4216.8
QD1	82	PHE	HZ	775.7
QD1	82	PHE	QR	4254.0*5
QD1	85	LEU	QD1	2572.0
QD2	82	PHE	QR	6614.0*5
QD2	85	LEU	QD1	11617.2
QD2	85	LEU	QD2	5251.0
QD2	91	ARG+	HA	10021.2
QD2	94	LEU	HB3	6996.0
QD2	94	LEU	HG	23444.4
QD2	94	LEU	QD1	20770.0
QD2	95	ILE	HA	864.4
QD2	95	ILE	HG12	2687.2
QD2	95	ILE	QD1	23030.0
69	THR			
HN	69	THR	HA	2670.0
HN	70	ASN	HN	20420.0
HA	69	THR	HB	11365.2
HA	69	THR	QG2	40412.4
HA	84	GLY	HA2	9735.6
HA	85	LEU	HN	3643.0
HB	69	THR	QG2	14742.0
QG2	86	LYS+	HA	21747.6
70	ASN			
HN	70	ASN	HA	4210.0
HN	70	ASN	HB2	6146.0
HN	71	PRO	HA	1673.0
HN	71	PRO	HD2	2523.0
HN	71	PRO	HD3	5713.0
HA	70	ASN	HB2	24259.2
HA	70	ASN	HB3	27426.0
HA	71	PRO	HG2	2374.0
HA	71	PRO	HG3	1474.2
HA	71	PRO	HD2	38379.6
HA	71	PRO	HD3	93390.0
HA	72	TML	HN	1533.0
HA	84	GLY	HA1	12516.0
HA	84	GLY	HA2	19395.6
HB2	73	LYS+	HN	1473.0
HB2	73	LYS+	HB2	6103.4
HB3	73	LYS+	HB3	15262.8
71	PRO			
HA	71	PRO	HB2	41748.0
HA	71	PRO	HB3	33200.0
HA	71	PRO	HG2	9480.0
HA	71	PRO	HG3	22495.2
HA	71	PRO	HD2	5811.1
HA	71	PRO	HD3	8450.4
HA	73	LYS+	HN	5510.0
HA	74	TYR	HN	2076.0
HA	74	TYR	HB2	7034.2
HA	74	TYR	HB3	8618.4
HA	75	ILE	HG12	10382.4
HA	78	THR	QG2	4137.0
HB2	71	PRO	HG2	16531.2
HB2	71	PRO	HG3	20563.2
HB2	71	PRO	HD2	34532.4
HB2	71	PRO	HD3	2756.9
HB2	72	TML	HN	20620.0
HB2	78	THR	QG2	31206.0
HB3	71	PRO	HG2	17380.0
HB3	71	PRO	HG3	18540.0
HB3	71	PRO	HD2	7137.5
HB3	71	PRO	HD3	5453.3
HB3	72	TML	HN	3206.0
HB3	78	THR	QG2	8912.4
HG2	71	PRO	HD2	16909.2
HG2	71	PRO	HD3	17505.6
HG2	82	PHE	QR	1973.6*5

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HG3	71	PRO	HD2	20252.4
HG3	71	PRO	HD3	20874.0
HD2	72	TML	HN	5365.0
HD2	84	GLY	HA1	10852.8
HD2	84	GLY	HA2	10189.2
HD3	72	TML	HN	579.0
HD3	82	PHE	QR	764.4*5
HD3	84	GLY	HA1	22722.0
HD3	84	GLY	HA2	25124.4
72 TML				
HN	72	TML	HA	836.0
HN	72	TML	HB2	7012.0
HN	72	TML	HB3	5867.0
HN	73	LYS+	HN	13320.0
HN	74	TYR	HN	4520.0
HN	78	THR	QG2	10270.0
HA	72	TML	HB2	11870.0
HA	72	TML	HB3	4946.8
HA	73	LYS+	HN	589.0
HA	78	THR	HN	106.0
HB2	72	TML	HE2	6304.0
HB3	72	TML	QQH	21140.0
HG2	72	TML	HE2	11360.0
HG2	72	TML	QQH	21820.0
HG2	73	LYS+	HN	9328.0
HG3	72	TML	HE2	9540.0
HE2	72	TML	QQH	38750.0
QQH	81	ALA	HA	17230.0
QQH	81	ALA	QB	10140.0
QQH	82	PHE	HN	5005.0
73 LYS+				
HN	73	LYS+	HB2	31710.0
HN	73	LYS+	HB3	26370.0
HN	73	LYS+	HG2	5077.0
HN	73	LYS+	HG3	2888.0
HN	73	LYS+	HD2	5259.0
HN	74	TYR	HN	49880.0
HN	75	ILE	HN	13110.0
HA	73	LYS+	HB2	38396.4
HA	73	LYS+	HB3	13246.8
HA	73	LYS+	HG2	16228.8
HA	73	LYS+	HG3	20017.2
HA	73	LYS+	HD2	7376.0
HA	73	LYS+	HE2	3612.0
HB2	73	LYS+	HE2	21848.4
HB2	74	TYR	HN	5219.0
HB3	73	LYS+	HE2	880.3
HB3	74	TYR	HN	13220.0
HG2	73	LYS+	HE2	9547.0
HD2	73	LYS+	HE2	57615.6
74 TYR				
HN	75	ILE	HN	13170.0
HA	74	TYR	HB2	21000.0
HA	74	TYR	HB3	11844.0
HA	74	TYR	CG	4321.8*2
HB2	74	TYR	CG	14460.6*2
HB3	74	TYR	CG	13494.6*2
HB3	75	ILE	HG12	18211.2
CG	74	TYR	CZ	24985.0*2*2
CG	75	ILE	HN	2551.5*2
CG	75	ILE	HB	3631.0*2
CG	75	ILE	QG2	1148.3*2
CG	75	ILE	HG13	17304.0*2
CG	75	ILE	QD1	13108.2*2
CZ	75	ILE	HG13	682.5*2
CZ	75	ILE	QD1	2047.9*2
75 ILE				
HN	75	ILE	HB	14770.0
HN	75	ILE	QG2	6691.0
HN	75	ILE	HG12	4216.0
HN	75	ILE	HG13	11310.0
HN	75	ILE	QD1	6055.0
HN	78	THR	QG2	13240.0
HA	75	ILE	QG2	12398.4
HA	75	ILE	HG12	11583.6
HA	75	ILE	QD1	5547.4
HB	78	THR	HB	40084.8
QG2	75	ILE	QD1	60940.0
QG2	78	THR	HA	7623.0
QG2	78	THR	HB	31441.2
76 PRO				
HA	76	PRO	HB2	18463.2
HA	76	PRO	HB3	107520.0
HA	76	PRO	HG2	17623.2
HA	76	PRO	HD2	5096.3
HA	77	GLY	HN	2668.0
HB3	76	PRO	HG2	330792.0
HB3	76	PRO	HD2	62739.6
HG2	76	PRO	HD2	82454.4
77 GLY				
HN	77	GLY	HA1	993.0
HN	78	THR	HN	321.0
HN	78	THR	QG2	16590.0
78 THR				
HN	78	THR	HB	5683.0
HN	78	THR	QG2	70850.0
HA	78	THR	HB	29576.4
HA	78	THR	QG2	17833.2
HB	78	THR	QG2	297864.0
QG2	79	LYS+	HN	7656.0
QG2	80	ALA	HN	5867.0
79 LYS+				
HN	79	LYS+	HG3	6735.0
HN	79	LYS+	HD2	2485.0
HN	79	LYS+	HE3	2193.0
HN	80	ALA	HN	10250.0
HB2	79	LYS+	HG2	38700.0
HB2	79	LYS+	HG3	17650.0
HB2	79	LYS+	HE3	3087.0
HB3	79	LYS+	HG2	10140.0
HB3	79	LYS+	HG3	6171.0
HB3	79	LYS+	HE3	4340.0
HG2	79	LYS+	HE3	17830.0
HG2	80	ALA	HN	5643.0
HG3	79	LYS+	HD2	16720.0
HG3	79	LYS+	HE3	38350.0
HG3	80	ALA	HN	14060.0
HG3	80	ALA	HA	1365.0
HD2	79	LYS+	HE3	50490.0
80 ALA				
HN	80	ALA	HA	12840.0
HN	80	ALA	QB	23040.0
HA	80	ALA	QB	11830.0
HA	81	ALA	HN	52050.0
HA	81	ALA	HA	386.0
HA	82	PHE	HN	964.0
81 ALA				
HN	81	ALA	HA	12160.0
HN	81	ALA	QB	33420.0
HN	82	PHE	HN	670.0
HA	81	ALA	QB	90828.0
HA	82	PHE	HN	15090.0
82 PHE				
HN	82	PHE	HB2	5356.0
HZ	82	PHE	QR	24860.0*5
HZ	84	GLY	HA1	4652.0

HZ	85	LEU	HN	2952.0
HZ	85	LEU	HA	3272.6
HZ	85	LEU	HB3	37580.0
HZ	85	LEU	HG	10130.4
HZ	85	LEU	QD1	12900.0
HZ	85	LEU	QD2	26120.0
QR	84	GLY	HA1	3922.8*5
QR	84	GLY	HA2	1953.8*5
QR	85	LEU	HN	2298.0*5
QR	85	LEU	HA	1137.7*5
QR	85	LEU	HB3	3596.9*5
QR	85	LEU	HG	4516.0*5
QR	85	LEU	QD1	4538.0*5
QR	85	LEU	QD2	1530.0*5
83	GLY			
HN	83	GLY	HA2	5407.3
HA2	85	LEU	HN	955.0
84	GLY			
HA1	85	LEU	HN	6531.0
HA2	85	LEU	HN	8510.0
85	LEU			
HN	85	LEU	HB2	10890.0
HN	85	LEU	HB3	4044.0
HN	85	LEU	HG	17150.0
HN	85	LEU	QD1	4507.0
HN	85	LEU	QD2	2021.0
HA	85	LEU	HB2	22369.2
HA	85	LEU	HB3	16514.4
HA	85	LEU	HG	27837.6
HA	85	LEU	QD1	10466.4
HA	85	LEU	QD2	41882.4
HB2	85	LEU	QD1	9752.4
HB3	85	LEU	QD1	27115.2
HB3	85	LEU	QD2	41420.4
HG	85	LEU	QD1	65226.0
QD1	91	ARG+	HA	26000.0
QD1	94	LEU	HG	21378.0
QD2	94	LEU	QD2	2210.9
86	LYS+			
HN	86	LYS+	HA	376.0
HN	86	LYS+	HB2	6640.0
HN	86	LYS+	HB3	10320.0
HN	86	LYS+	HG2	13910.0
HN	87	LYS+	HN	20940.0
HA	86	LYS+	HB2	6252.1
HA	86	LYS+	HB3	27711.6
HA	86	LYS+	HG2	17371.2
HA	86	LYS+	HG3	31021.2
HA	86	LYS+	HD2	12087.6
HA	86	LYS+	HD3	13246.8
HA	86	LYS+	HE2	6909.0
HB2	87	LYS+	HN	5364.0
HB3	87	LYS+	HN	5807.0
87	LYS+			
HN	87	LYS+	HA	2873.0
HN	87	LYS+	HB2	6907.0
HN	87	LYS+	HB3	25880.0
HN	87	LYS+	HG2	13260.0
HN	87	LYS+	HG3	10600.0
HA	87	LYS+	HB2	43528.8
HA	87	LYS+	HB3	16816.8
HB2	90	ASP-	HN	5394.0
HB3	89	LYS+	HN	33370.0
HB3	90	ASP-	HN	24440.0
88	GLU-			
HN	89	LYS+	HN	12840.0
89	LYS+			
HN	89	LYS+	HA	13580.0
HN	89	LYS+	HB2	34610.0
HN	89	LYS+	HG2	14300.0
HN	89	LYS+	HD3	24960.0
HN	90	ASP-	HN	12330.0
HA	89	LYS+	HB2	30660.0
HA	89	LYS+	HB3	18660.0
HA	89	LYS+	HG2	18958.8
HA	89	LYS+	HG3	26073.6
HA	89	LYS+	HD2	15808.8
HA	89	LYS+	HD3	27980.4
HA	90	ASP-	HN	4185.0
HA	92	ASN	HN	4722.0
HA	93	ASP-	HN	2181.0
HB2	90	ASP-	HN	17430.0
HB3	90	ASP-	HN	12360.0
HG3	90	ASP-	HN	8872.0
90	ASP-			
HN	90	ASP-	HA	17730.0
HN	90	ASP-	HB2	15290.0
HN	90	ASP-	HB3	6503.0
HN	91	ARG+	HN	21430.0
HN	92	ASN	HN	1421.0
HA	90	ASP-	HB2	15859.2
HA	90	ASP-	HB3	19420.8
HA	91	ARG+	HN	3970.0
HA	93	ASP-	HN	12020.0
HB2	91	ARG+	HN	6921.0
HB3	91	ARG+	HN	11950.0
91	ARG+			
HN	91	ARG+	HA	11100.0
HN	91	ARG+	HB2	19960.0
HN	91	ARG+	HB3	19850.0
HN	91	ARG+	HG2	9066.0
HN	92	ASN	HN	9949.0
HA	91	ARG+	HB2	21361.2
HA	91	ARG+	HB3	13880.0
HA	91	ARG+	HG2	58086.0
HA	91	ARG+	HD2	3473.4
HA	92	ASN	HN	4820.0
HA	94	LEU	HN	3891.0
HA	94	LEU	HB2	8408.4
HA	94	LEU	HB3	46317.6
HA	95	ILE	QD1	9517.2
HB2	91	ARG+	HG2	84840.0
HB2	92	ASN	HN	4686.0
HB2	95	ILE	HG12	9307.2
HB3	91	ARG+	HG2	27274.8
HB3	92	ASN	HN	12690.0
HB3	95	ILE	QD1	13582.8
92	ASN			
HN	92	ASN	HA	1609.0
HN	92	ASN	HB3	17780.0
HN	94	LEU	HB3	2868.0
HA	92	ASN	HB3	20302.8
HA	93	ASP-	HN	1555.0
HA	95	ILE	QD1	9433.2
HB3	93	ASP-	HN	16720.0
93	ASP-			
HN	93	ASP-	HA	7747.0
HN	93	ASP-	HB2	23990.0
HN	93	ASP-	HB3	5800.0
HN	94	LEU	HN	19390.0
HA	93	ASP-	HB2	17211.6
HA	93	ASP-	HB3	10060.0
HA	94	LEU	HN	4062.0
HB2	94	LEU	HN	5835.0
HB3	94	LEU	HN	10250.0
94	LEU			

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HN	94	LEU	HA	9368.0
HN	94	LEU	HB3	34510.0
HN	94	LEU	HG	5513.0
HN	94	LEU	QD1	4805.0
HN	94	LEU	QD2	6047.0
HN	95	ILE	HN	14000.0
HA	94	LEU	HB2	8412.0
HA	94	LEU	HB3	13120.8
HA	94	LEU	HG	12154.8
HA	94	LEU	QD1	6930.8
HA	94	LEU	QD2	25980.0
HA	95	ILE	HN	4580.0
HA	97	TYR	HN	2713.0
HB2	94	LEU	HG	127700.0
HB2	94	LEU	QD1	23116.8
HB2	94	LEU	QD2	12776.4
HB2	95	ILE	HN	30780.0
HB3	94	LEU	HG	49098.0
HB3	94	LEU	QD1	32785.2
HB3	94	LEU	QD2	30181.2
HB3	95	ILE	HN	2349.0
HB3	95	ILE	HG12	8828.4
HG	94	LEU	QD1	36346.8
HG	94	LEU	QD2	28719.6
HG	95	ILE	HN	15900.0
HG	95	ILE	HA	7594.4
QD1	97	TYR	HN	835.0
QD1	98	LEU	HN	9146.0
QD1	98	LEU	HG	13188.0
QD1	98	LEU	QD1	12079.2
QD2	98	LEU	QD1	3079.4
95	ILE			
HN	95	ILE	HA	14550.0
HN	95	ILE	HB	37930.0
HN	95	ILE	QG2	11160.0
HN	95	ILE	HG12	18640.0
HN	95	ILE	QD1	17680.0
HN	96	THR	HN	8409.0
HA	95	ILE	HB	11986.8
HA	95	ILE	QG2	24864.0
HA	95	ILE	HG12	12734.4
HA	95	ILE	QD1	4210.0
HA	96	THR	HN	3862.0
HA	98	LEU	HN	12300.0
HA	98	LEU	HB2	16880.0
HA	98	LEU	HB3	16060.0
HA	98	LEU	QD1	1963.1
HA	98	LEU	QD2	1945.4
HA	99	LYS+	HN	2217.0
HB	95	ILE	QG2	37161.6
HB	95	ILE	HG12	36900.0
HB	95	ILE	QD1	50005.2
HB	96	THR	HN	20060.0
QG2	95	ILE	QD1	53146.8
QG2	96	THR	HN	11840.0
QG2	96	THR	HA	1305.4
QG2	98	LEU	HB2	27070.0
QG2	99	LYS+	HN	1928.0
QG2	99	LYS+	HB2	30928.8
QG2	99	LYS+	HB3	7320.6
HG12	95	ILE	QD1	22965.6
HG12	98	LEU	QD2	8946.0
QD1	96	THR	HN	2372.0
96	THR			
HN	96	THR	HA	8831.0
HN	97	TYR	HN	14760.0
HA	96	THR	HB	12776.4
HA	96	THR	QG2	33310.0
HA	97	TYR	HN	3204.0
HA	99	LYS+	HN	1087.0
HA	99	LYS+	HB2	6036.2
HA	99	LYS+	HB3	31458.0
HB	96	THR	QG2	75616.8
QG2	97	TYR	HN	7808.0
QG2	97	TYR	HA	18916.8
97	TYR			
HN	97	TYR	HA	20590.0
HN	97	TYR	HB2	16630.0
HN	97	TYR	HB3	14840.0
HN	98	LEU	HN	24480.0
HA	97	TYR	HB2	53894.4
HA	97	TYR	HB3	13381.2
HA	98	LEU	HN	5489.0
HA	100	LYS+	HN	4587.0
HA	101	ALA	HN	2678.0
HB2	98	LEU	HN	2754.0
HB3	98	LEU	HN	20340.0
HD1	97	TYR	HE1	1700.0
HD1	97	TYR	HE2	9697.0
HE1	97	TYR	HD2	3508.0
HE2	97	TYR	HD2	8246.3
98	LEU			
HN	98	LEU	HA	11220.0
HN	98	LEU	HB2	34480.0
HN	98	LEU	HB3	12120.0
HN	98	LEU	HG	4398.0
HN	98	LEU	QD1	4309.0
HN	98	LEU	QD2	572.0
HN	99	LYS+	HN	21910.0
HN	101	ALA	QB	1967.0
HA	98	LEU	HB2	19303.2
HA	98	LEU	HB3	4032.8
HA	98	LEU	QD1	5180.3
HA	98	LEU	QD2	24343.2
HA	99	LYS+	HN	3723.0
HA	100	LYS+	HN	3548.0
HA	101	ALA	HN	6848.0
HA	101	ALA	QB	26830.0
HA	102	SER	HN	3996.0
HB2	98	LEU	QD1	74410.0
HB2	98	LEU	QD2	61311.6
HB2	99	LYS+	HN	14390.0
HB3	98	LEU	QD1	37210.0
HB3	98	LEU	QD2	32432.4
HB3	99	LYS+	HN	19630.0
HG	98	LEU	QD1	16580.0
HG	98	LEU	QD2	20714.4
QD1	99	LYS+	HN	1599.0
99	LYS+			
HN	99	LYS+	HA	17400.0
HN	99	LYS+	HB2	22070.0
HN	99	LYS+	HB3	47840.0
HN	99	LYS+	HG2	7700.0
HN	99	LYS+	HG3	10920.0
HN	100	LYS+	HN	15860.0
HA	99	LYS+	HB2	33465.6
HA	99	LYS+	HB3	11104.8
HA	99	LYS+	HG2	21450.0
HA	99	LYS+	HG3	18340.0
HA	99	LYS+	HD2	13040.0
HA	100	LYS+	HN	4627.0
HB2	99	LYS+	HG2	20538.0
HB2	99	LYS+	HG3	16926.0
HB2	99	LYS+	HD2	14977.2
HB2	99	LYS+	HD3	45301.2
HB3	99	LYS+	HG2	11650.8

HB3	99	LYS+	HG3	27140.4
HB3	99	LYS+	HD2	16245.6
HB3	99	LYS+	HD3	21546.0
HB3	100	LYS+	HN	18840.0
HG2	99	LYS+	HD2	10718.4
HG2	99	LYS+	HD3	11010.0
HG2	100	LYS+	HG2	10978.8
HG3	99	LYS+	HD3	30860.0
HG3	100	LYS+	HN	9618.0
100 LYS+				
HN	100	LYS+	HA	18140.0
HN	100	LYS+	HB2	29630.0
HN	100	LYS+	HB3	18660.0
HN	100	LYS+	HG2	34920.0
HN	100	LYS+	HD2	4260.0
HN	101	ALA	HN	38170.0
HN	101	ALA	QB	6212.0
HN	102	SER	HN	4045.0
HA	100	LYS+	HB2	13790.0
HA	100	LYS+	HB3	18910.0
HA	100	LYS+	HG2	29500.8
HA	101	ALA	HN	3551.0
HA	103	GLU-	HB2	1634.0
HB2	100	LYS+	HG2	170604.0
HB2	101	ALA	HN	8669.0
HB3	101	ALA	HN	9215.0
HG2	100	LYS+	HD2	109284.0
HG2	100	LYS+	HE2	46779.6
HG2	101	ALA	HN	4147.0
HD2	100	LYS+	HE2	20412.0
101 ALA				
HN	101	ALA	HA	12190.0
HN	101	ALA	QB	67320.0
HN	102	SER	HN	19940.0
HN	103	GLU-	HN	1856.0
HA	101	ALA	QB	79111.2
HA	102	SER	HN	6160.0
HA	103	GLU-	HN	5469.0
QB	102	SER	HN	19600.0
102 SER				
HN	102	SER	HA	6285.0
HN	102	SER	HB2	10560.0
HN	103	GLU-	HN	24380.0
HA	102	SER	HB2	5993.0
103 GLU-				
HN	103	GLU-	HA	21050.0
HN	103	GLU-	HB2	34620.0
HN	103	GLU-	HB3	16390.0
HN	103	GLU-	HG2	3696.0
HN	103	GLU-	HG3	3426.0
HA	103	GLU-	HB2	37390.0
HA	103	GLU-	HB3	12350.0
HA	103	GLU-	HG2	1159.0
HA	103	GLU-	HG3	1023.0
HB2	103	GLU-	HG2	21302.4
HB2	103	GLU-	HG3	82790.4
HB3	103	GLU-	HG2	88032.0
HB3	103	GLU-	HG3	45864.0

1D NOE intensities

18 HES				
HA	18	HES	HD1	17700.0
HB2	18	HES	HD1	18100.0
HB3	18	HES	HD1	17600.0
HD1	19	THR	HN	14400.0
HD1	31	ASN	HA	9800.0
67 TYR				
HH	71	PRO	HG3	36700.0
HH	71	PRO	HB2	81400.0
HH	71	PRO	HB3	82200.0

PART II

Irrelevant NOE constraints

HN	PHE	-3	HA	PHE	-3
HN	PHE	-3	CG	PHE	-3
HA	PHE	-3	HB3	PHE	-3
HA	PHE	-3	CG	PHE	-3
HB2	PHE	-3	CG	PHE	-3
HB3	PHE	-3	CG	PHE	-3
CG	PHE	-3	CZ	PHE	-3
CG	PHE	-3	HZ	PHE	-3
CZ	PHE	-3	HZ	PHE	-3
HN	LYS+	-2	HA	LYS+	-2
HA	LYS+	-2	HB3	LYS+	-2
HG2	LYS+	-2	HE2	LYS+	-2
HD2	LYS+	-2	HE2	LYS+	-2
HN	ALA	-1	HA	ALA	-1
HA	ALA	-1	QB	ALA	-1
HN	GLY	1	HA1	GLY	1
HA	SER	2	HB2	SER	2
HA	ALA	3	QB	ALA	3
HN	LYS+	4	HA	LYS+	4
HA	LYS+	4	HB2	LYS+	4
HA	LYS+	4	HN	LYS+	5
HA	LYS+	5	HB2	LYS+	5
HA	LYS+	5	HN	GLY	6
HB3	LYS+	5	HG2	LYS+	5
HN	GLY	6	HA1	GLY	6
HN	GLY	6	HA2	GLY	6
HA	ALA	7	QB	ALA	7
HN	THR	8	HA	THR	8
HN	THR	8	QG2	THR	8
HA	THR	8	HB	THR	8
HB	THR	8	QG2	THR	8
HA	LEU	9	HB2	LEU	9
HA	LEU	9	HN	PHE	10
HB2	LEU	9	QD1	LEU	9
HB3	LEU	9	QD2	LEU	9
HA	PHE	10	HN	LYS+	11
HE1	PHE	10	HD2	PHE	10
HZ	PHE	10	HE2	PHE	10
HE2	PHE	10	HD2	PHE	10
HN	LYS+	11	HA	LYS+	11
HA	LYS+	11	HB2	LYS+	11
HA	LYS+	11	HN	THR	12
HN	THR	12	HA	THR	12
HA	THR	12	HN	ARG+	13
HN	ARG+	13	HA	ARG+	13
HA	ARG+	13	HB2	ARG+	13
HN	CYSS	14	HA	CYSS	14
HA	CYSS	14	HB2	CYSS	14
HA	LEU	15	HB3	LEU	15
HA	LEU	15	HN	GLN	16
HG	LEU	15	QD1	LEU	15
HG	LEU	15	QD2	LEU	15
HN	GLN	16	HA	GLN	16
HG2	GLN	16	HE21	GLN	16
HG2	GLN	16	HE22	GLN	16
HG3	GLN	16	HE21	GLN	16
HN	CYSS	17	HA	CYSS	17
HA	CYSS	17	HB2	CYSS	17
HA	CYSS	17	HN	HES	18

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HN	HES	18	-	HA	HES	18	HB2	ASN	31	-	HD21	ASN	31
HA	HES	18	-	HB2	HES	18	HB2	ASN	31	-	HD22	ASN	31
HB2	HES	18	-	HD1	HES	18	HB3	ASN	31	-	HD21	ASN	31
HB3	HES	18	-	HD1	HES	18	HB3	ASN	31	-	HD22	ASN	31
HAP71	HES	18	-	HAP72	HES	18	HN	LEU	32	-	HA	LEU	32
HAP71	HES	18	-	HBP73	HES	18	HA	LEU	32	-	HB2	LEU	32
HAP72	HES	18	-	HBP74	HES	18	HB2	LEU	32	-	HG	LEU	32
QM8	HES	18	-	HDM	HES	18	HB2	LEU	32	-	QD1	LEU	32
HDM	HES	18	-	QM1	HES	18	HB2	LEU	32	-	QD2	LEU	32
QM1	HES	18	-	QT2	HES	18	HB3	LEU	32	-	HG	LEU	32
HAM	HES	18	-	QM3	HES	18	HB3	LEU	32	-	QD2	LEU	32
QM3	HES	18	-	HT4A	HES	18	HG	LEU	32	-	QD1	LEU	32
QM3	HES	18	-	QT4	HES	18	HG	LEU	32	-	QD2	LEU	32
HBM	HES	18	-	QM5	HES	18	HN	HIS	33	-	HA	HIS	33
HAP61	HES	18	-	HBP63	HES	18	HA	HIS	33	-	HB2	HIS	33
HN	THR	19	-	HA	THR	19	HB2	HIS	33	-	HD2	HIS	33
HB	THR	19	-	QG2	THR	19	HB3	HIS	33	-	HD2	HIS	33
HA	VAL	20	-	QG1	VAL	20	HN	GLY	34	-	HA2	GLY	34
HA	VAL	20	-	QG2	VAL	20	HN	ILE	35	-	HA	ILE	35
HB	VAL	20	-	QG1	VAL	20	HA	ILE	35	-	QG2	ILE	35
HB	VAL	20	-	QG2	VAL	20	HA	ILE	35	-	HN	PHE	36
HA	GLU-	21	-	HB3	GLU-	21	HB	ILE	35	-	QG2	ILE	35
HA	GLU-	21	-	HG2	GLU-	21	HB	ILE	35	-	HG12	ILE	35
HA	GLU-	21	-	HG3	GLU-	21	HB	ILE	35	-	HG13	ILE	35
HA	LYS+	22	-	HB2	LYS+	22	QG2	ILE	35	-	HG12	ILE	35
HB2	LYS+	22	-	HG2	LYS+	22	HG12	ILE	35	-	QD1	ILE	35
HB3	LYS+	22	-	HG3	LYS+	22	HG13	ILE	35	-	QD1	ILE	35
HG2	LYS+	22	-	HD2	LYS+	22	HN	PHE	36	-	HA	PHE	36
HG2	LYS+	22	-	HE3	LYS+	22	HA	PHE	36	-	CG	PHE	36
HG3	LYS+	22	-	HD2	LYS+	22	HA	PHE	36	-	CZ	PHE	36
HD2	LYS+	22	-	HE3	LYS+	22	HB2	PHE	36	-	CG	PHE	36
HN	GLY	23	-	HA2	GLY	23	HB3	PHE	36	-	CG	PHE	36
HN	GLY	24	-	HA1	GLY	24	CG	PHE	36	-	CZ	PHE	36
HN	GLY	24	-	HA2	GLY	24	CG	PHE	36	-	HZ	PHE	36
HA	PRO	25	-	HB3	PRO	25	CZ	PHE	36	-	HZ	PHE	36
HA	PRO	25	-	HN	HIS	26	HN	GLY	37	-	HA1	GLY	37
HB3	PRO	25	-	HG2	PRO	25	HN	GLY	37	-	HA2	GLY	37
HB3	PRO	25	-	HG3	PRO	25	HA2	GLY	37	-	HN	ARG+	38
HG3	PRO	25	-	HD2	PRO	25	HA	ARG+	38	-	HB3	ARG+	38
HN	HIS	26	-	HA	HIS	26	HA	ARG+	38	-	HG2	ARG+	38
HN	HIS	26	-	HB3	HIS	26	HN	GLN	39	-	HA	GLN	39
HA	HIS	26	-	HB2	HIS	26	HA	GLN	39	-	HB3	GLN	39
HB2	HIS	26	-	HD2	HIS	26	HN	SER	40	-	HA	SER	40
HN	LYS+	27	-	HA	LYS+	27	HN	GLN	42	-	HA	GLN	42
HA	LYS+	27	-	HB2	LYS+	27	HA	GLN	42	-	HB3	GLN	42
HA	LYS+	27	-	HN	VAL	28	HA	GLN	42	-	HN	ALA	43
HB2	LYS+	27	-	HG3	LYS+	27	HB2	GLN	42	-	HG2	GLN	42
HB3	LYS+	27	-	HG3	LYS+	27	HB2	GLN	42	-	HG3	GLN	42
HG3	LYS+	27	-	HD2	LYS+	27	HB3	GLN	42	-	HG2	GLN	42
HD2	LYS+	27	-	HE2	LYS+	27	HB3	GLN	42	-	HG3	GLN	42
HD2	LYS+	27	-	E3	LYS+	27	HG2	GLN	42	-	HE21	GLN	42
HD3	LYS+	27	-		LYS+	27	HG3	GLN	42	-	HE21	GLN	42
HN	VAL	28	-		VAL	28	HG3	GLN	42	-	HE22	GLN	42
HA	VAL	28	-	h.	VAL	28	HN	ALA	43	-	HA	ALA	43
HA	VAL	28	-	HN	GLY	29	HA	ALA	43	-	QB	ALA	43
HB	VAL	28	-	QG1	VAL	28	QB	ALA	43	-	HN	GLU-	44
HB	VAL	28	-	QG2	VAL	28	HN	GLU-	44	-	HA	GLU-	44
HN	GLY	29	-	HA1	GLY	29	HA	GLU-	44	-	HG3	GLU-	44
HA	PRO	30	-	HB2	PRO	30	HA	GLU-	44	-	HN	GLY	45
HA	PRO	30	-	HB3	PRO	30	HN	GLY	45	-	HA1	GLY	45
HA	PRO	30	-	HG2	PRO	30	HN	GLY	45	-	HA2	GLY	45
HA	PRO	30	-	HG3	PRO	30	HA1	GLY	45	-	HN	TYR	46
HA	PRO	30	-	HD2	PRO	30	HN	TYR	46	-	HA	TYR	46
HB2	PRO	30	-	HG3	PRO	30	HA	TYR	46	-	HB3	TYR	46
HB3	PRO	30	-	HG3	PRO	30	HB2	TYR	46	-	HD1	TYR	46
HG3	PRO	30	-	HD2	PRO	30	HB3	TYR	46	-	HD1	TYR	46
HN	ASN	31	-	HA	ASN	31	HD1	TYR	46	-	HE1	TYR	46
HA	ASN	31	-	HB3	ASN	31	HD1	TYR	46	-	HE2	TYR	46

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HE1	TYR	46	-	HD2	TYR	46	HB3	ASN	63	-	HD22	ASN	63
HE2	TYR	46	-	HD2	TYR	46	HN	MET	64	-	HA	MET	64
HE2	TYR	46	-	HH	TYR	46	HN	SER	65	-	HA	SER	65
HN	SER	47	-	HA	SER	47	HA	SER	65	-	HB3	SER	65
HN	TYR	48	-	HA	TYR	48	HN	GLU-	66	-	HA	GLU-	66
HA	TYR	48	-	HB3	TYR	48	HA	GLU-	66	-	HB3	GLU-	66
HB2	TYR	48	-	HD1	TYR	48	HA	GLU-	66	-	HN	TYR	67
HB2	TYR	48	-	HD2	TYR	48	HB2	GLU-	66	-	HG2	GLU-	66
HB3	TYR	48	-	HD1	TYR	48	HB3	GLU-	66	-	HG2	GLU-	66
HB3	TYR	48	-	HD2	TYR	48	HN	TYR	67	-	HA	TYR	67
HD1	TYR	48	-	HE1	TYR	48	HA	TYR	67	-	HB2	TYR	67
HD1	TYR	48	-	HH	TYR	48	HA	TYR	67	-	HB3	TYR	67
HE1	TYR	48	-	HD2	TYR	48	HD1	TYR	67	-	HE2	TYR	67
HE1	TYR	48	-	HH	TYR	48	HN	LEU	68	-	HA	LEU	68
HE2	TYR	48	-	HH	TYR	48	HB2	LEU	68	-	QD1	LEU	68
HN	THR	49	-	HA	THR	49	HB2	LEU	68	-	QD2	LEU	68
HB	THR	49	-	QG2	THR	49	HB3	LEU	68	-	QD1	LEU	68
HN	ASP-	50	-	HA	ASP-	50	HG	LEU	68	-	QD1	LEU	68
HA	ASP-	50	-	HB2	ASP-	50	HG	LEU	68	-	QD2	LEU	68
HN	ALA	51	-	HA	ALA	51	HN	THR	69	-	HA	THR	69
HA	ALA	51	-	QB	ALA	51	HA	THR	69	-	HB	THR	69
HA	ALA	51	-	HN	ASN	52	HB	THR	69	-	QG2	THR	69
HN	ASN	52	-	HA	ASN	52	HN	ASN	70	-	HA	ASN	70
HA	ASN	52	-	HB3	ASN	52	HA	PRO	71	-	HB2	PRO	71
HB2	ASN	52	-	HD21	ASN	52	HA	PRO	71	-	HB3	PRO	71
HB2	ASN	52	-	HD22	ASN	52	HA	PRO	71	-	HG2	PRO	71
HB3	ASN	52	-	HD21	ASN	52	HA	PRO	71	-	HG3	PRO	71
HB3	ASN	52	-	HD22	ASN	52	HA	PRO	71	-	HD2	PRO	71
HN	ILE	53	-	HA	ILE	53	HA	PRO	71	-	HD3	PRO	71
HA	ILE	53	-	HB	ILE	53	HB2	PRO	71	-	HG2	PRO	71
HA	ILE	53	-	HG13	ILE	53	HB2	PRO	71	-	HG3	PRO	71
HA	ILE	53	-	HN	LYS+	54	HB2	PRO	71	-	HD2	PRO	71
HB	ILE	53	-	QG2	ILE	53	HB2	PRO	71	-	HD3	PRO	71
HB	ILE	53	-	HG12	ILE	53	HB3	PRO	71	-	HG2	PRO	71
HG12	ILE	53	-	QD1	ILE	53	HB3	PRO	71	-	HG3	PRO	71
HG13	ILE	53	-	QD1	ILE	53	HB3	PRO	71	-	HD2	PRO	71
HN	LYS+	55	-	HA	LYS+	55	HB3	PRO	71	-	HD3	PRO	71
HA	LYS+	55	-	HB3	LYS+	55	HG2	PRO	71	-	HD2	PRO	71
HA	LYS+	55	-	HG2	LYS+	55	HG2	PRO	71	-	HD3	PRO	71
HA	LYS+	55	-	HN	ASN	56	HG3	PRO	71	-	HD2	PRO	71
HA	ASN	56	-	HB3	ASN	56	HG3	PRO	71	-	HD3	PRO	71
HB2	ASN	56	-	HD22	ASN	56	HD3	PRO	71	-	HN	TML	72
HB3	ASN	56	-	HD22	ASN	56	HN	TML	72	-	HA	TML	72
HN	VAL	57	-	HA	VAL	57	HA	TML	72	-	HB2	TML	72
HA	VAL	57	-	HB	VAL	57	HA	TML	72	-	HB3	TML	72
HA	VAL	57	-	QG1	VAL	57	HA	TML	72	-	HN	LYS+	73
HA	VAL	57	-	QG2	VAL	57	HG2	TML	72	-	HE2	TML	72
HB	VAL	57	-	QG1	VAL	57	HG3	TML	72	-	HE2	TML	72
HB	VAL	57	-	QG2	VAL	57	HE2	TML	72	-	QQH	TML	72
HN	LEU	58	-	HA	LEU	58	HA	LYS+	73	-	HB3	LYS+	73
HA	LEU	58	-	HB3	LEU	58	HG2	LYS+	73	-	HE2	LYS+	73
HB2	LEU	58	-	QD2	LEU	58	HA	TYR	74	-	HB3	TYR	74
HB2	TRP	59	-	HD1	TRP	59	HA	TYR	74	-	CG	TYR	74
HB2	TRP	59	-	HE3	TRP	59	HB2	TYR	74	-	CG	TYR	74
HD1	TRP	59	-	HE1	TRP	59	HB3	TYR	74	-	CG	TYR	74
HE3	TRP	59	-	HZ3	TRP	59	CG	TYR	74	-	CZ	TYR	74
HE3	TRP	59	-	HH2	TRP	59	HN	ILE	75	-	QG2	ILE	75
HE1	TRP	59	-	HZ2	TRP	59	HA	ILE	75	-	QG2	ILE	75
HZ3	TRP	59	-	HZ2	TRP	59	HA	ILE	75	-	HG12	ILE	75
HZ3	TRP	59	-	HH2	TRP	59	HA	ILE	75	-	QD1	ILE	75
HZ2	TRP	59	-	HH2	TRP	59	HA	PRO	76	-	HB2	PRO	76
HN	GLU-	61	-	HA	GLU-	61	HA	PRO	76	-	HB3	PRO	76
HA	ASN	62	-	HB2	ASN	62	HA	PRO	76	-	HG2	PRO	76
HB2	ASN	62	-	HD21	ASN	62	HA	PRO	76	-	HD2	PRO	76
HB3	ASN	62	-	HD21	ASN	62	HA	PRO	76	-	HN	GLY	77
HB3	ASN	62	-	HD22	ASN	62	HB3	PRO	76	-	HG2	PRO	76
HN	ASN	63	-	HA	ASN	63	HB3	PRO	76	-	HD2	PRO	76
HB3	ASN	63	-	HD21	ASN	63	HG2	PRO	76	-	HD2	PRO	76

HN	GLY	77	HA1	GLY	77
HA	THR	78	QG2	THR	78
HB	THR	78	QG2	THR	78
HB2	LYS+	79	HG2	LYS+	79
HB2	LYS+	79	HG3	LYS+	79
HB3	LYS+	79	HG2	LYS+	79
HB3	LYS+	79	HG3	LYS+	79
HG3	LYS+	79	HD2	LYS+	79
HN	ALA	80	HA	ALA	80
HA	ALA	80	QB	ALA	80
HN	ALA	81	HA	ALA	81
HA	ALA	81	QB	ALA	81
HZ	PHE	82	QR	PHE	82
HN	GLY	83	HA2	GLY	83
HB2	LEU	85	QD1	LEU	85
HG	LEU	85	QD1	LEU	85
HN	LYS+	86	HA	LYS+	86
HA	LYS+	86	HB2	LYS+	86
HN	LYS+	87	HA	LYS+	87
HN	LYS+	89	HA	LYS+	89
HA	LYS+	89	HN	ASP-	90
HN	ASP-	90	HA	ASP-	90
HA	ASP-	90	HN	ARG+	91
HN	ARG+	91	HA	ARG+	91
HA	ARG+	91	HB3	ARG+	91
HA	ARG+	91	HN	ASN	92
HB3	ARG+	91	HG2	ARG+	91
HN	ASN	92	HA	ASN	92
HA	ASN	92	HN	ASP-	93
HN	ASP-	93	HA	ASP-	93
HA	ASP-	93	HB3	ASP-	93
HA	ASP-	93	HN	LEU	94
HN	LEU	94	HA	LEU	94
HA	LEU	94	HB2	LEU	94
HA	LEU	94	HB3	LEU	94
HA	LEU	94	HN	ILE	95
HB2	LEU	94	QD1	LEU	94
HB2	LEU	94	QD2	LEU	94
HG	LEU	94	QD1	LEU	94
HG	LEU	94	QD2	LEU	94
HN	ILE	95	HA	ILE	95
HA	ILE	95	HB	ILE	95
HA	ILE	95	QD1	ILE	95
HA	ILE	95	HN	THR	96
HB	ILE	95	QG2	ILE	95
HB	ILE	95	HG12	ILE	95
HG12	ILE	95	QD1	ILE	95
HN	THR	96	HA	THR	96
HA	THR	96	HB	THR	96
HA	THR	96	HN	TYR	97
HB	THR	96	QG2	THR	96
HA	TYR	97	HB3	TYR	97
HD1	TYR	97	HE1	TYR	97
HD1	TYR	97	HE2	TYR	97
HE1	TYR	97	HD2	TYR	97
HE2	TYR	97	HD2	TYR	97
HN	LEU	98	HA	LEU	98
HA	LEU	98	HB3	LEU	98
HA	LEU	98	HN	LYS+	99
HG	LEU	98	QD1	LEU	98
HG	LEU	98	QD2	LEU	98
HN	LYS+	99	HA	LYS+	99
HA	LYS+	99	HB3	LYS+	99
HA	LYS+	99	HN	LYS+	100
HB2	LYS+	99	HG2	LYS+	99
HB2	LYS+	99	HG3	LYS+	99
HB3	LYS+	99	HG2	LYS+	99
HB3	LYS+	99	HG3	LYS+	99
HG2	LYS+	99	HD2	LYS+	99
HG2	LYS+	99	HD3	LYS+	99
HG3	LYS+	99	HD3	LYS+	99
HN	LYS+	100	HA	LYS+	100
HA	LYS+	100	HB2	LYS+	100
HA	LYS+	100	HN	ALA	101
HD2	LYS+	100	HE2	LYS+	100
HN	ALA	101	HA	ALA	101
HA	ALA	101	QB	ALA	101
HN	SER	102	HA	SER	102
HA	SER	102	HB2	SER	102
HA	GLU-	103	HB3	GLU-	103
HA	GLU-	103	HG2	GLU-	103
HA	GLU-	103	HG3	GLU-	103
HB2	GLU-	103	HG2	GLU-	103

PART III

Hydrogen bond constraints

10 PHE				
HN	6	GLY	O	2.40
N	6	GLY	O	3.40
11 LYS+				
HN	7	ALA	O	2.40
N	7	ALA	O	3.40
12 THR				
HN	9	LEU	O	2.40
N	9	LEU	O	3.40
15 LEU				
HN	10	PHE	O	2.40
N	10	PHE	O	3.40
68 LEU				
HN	64	MET	O	2.40
N	64	MET	O	3.40
75 ILE				
HN	71	PRO	O	2.40
N	71	PRO	O	3.40
94 LEU				
HN	90	ASP-	O	2.40
N	90	ASP-	O	3.40
95 ILE				
HN	91	ARG+	O	2.40
N	91	ARG+	O	3.40
97 TYR				
HN	93	ASP-	O	2.40
N	93	ASP-	O	3.40
98 LEU				
HN	94	LEU	O	2.40
N	94	LEU	O	3.40
99 LYS+				
HN	95	ILE	O	2.40
N	95	ILE	O	3.40
101 ALA				
HN	97	TYR	O	2.40
N	97	TYR	O	3.40
102 SER				
HN	98	LEU	O	2.40
N	98	LEU	O	3.40
1 GLY				
HN	96	THR	OG1	2.40
N	96	THR	OG1	3.40
43 ALA				
HN	48	TYR	OH	2.40
N	48	TYR	OH	3.40
41 GLY				

HN	18	HES	O2A	2.40
N	18	HES	O2A	3.40
59	TRP			
HE1	18	HES	O2A	2.70
NE1	18	HES	O2A	3.70